
Why Do Transformers Fail to Forecast Time Series In-Context?

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Abstract

Time series forecasting (TSF) remains a challenging and largely unsolved problem in machine learning, despite significant recent efforts leveraging Large Language Models (LLMs), which predominantly rely on Transformer architectures. Empirical evidence consistently shows that even powerful Transformers often fail to outperform much simpler models, e.g., linear models, on TSF tasks; however, a rigorous theoretical understanding of this phenomenon remains limited. In this paper, we provide a theoretical analysis of Transformers’ limitations for TSF through the lens of In-Context Learning (ICL) theory. Specifically, under $AR(p)$ data, we establish that: (1) Linear Self-Attention (LSA) models *cannot* achieve lower expected MSE than classical linear models for in-context forecasting; (2) as the context length approaches to infinity, LSA asymptotically recovers the optimal linear predictor; and (3) under Chain-of-Thought (CoT) style inference, predictions collapse to the mean exponentially. We empirically validate these findings through carefully designed experiments. Our theory not only sheds light on several previously underexplored phenomena but also offers practical insights for designing more effective forecasting architectures. We hope our work encourages the broader research community to revisit the fundamental theoretical limitations of TSF and to critically evaluate the direct application of increasingly sophisticated architectures without deeper scrutiny. See full version at: <https://arxiv.org/abs/2510.09776>.

“The only thing we know about the future is that it will be different.”

— Peter Drucker

1 Introduction

Time series forecasting (TSF), a fundamental and longstanding challenge in machine learning, involves predicting future observations based on historical data [BD02, BJRL15, DGH06, Ham20]. TSF has broad applicability across diverse fields such as electronic health records, traffic analysis, energy consumption, and financial market predictions [MJK15, MMM23]. In contrast, Transformers [VSP⁺17] have emerged as a cornerstone architecture in modern deep learning, achieving groundbreaking success across a wide array of sequence modeling tasks, including language modeling [HLG⁺24, JKL⁺24, GDJ⁺24, YLY⁺25, GYZ⁺25], computer vision [DBK⁺21, PX23, MGA⁺24], visual-language modeling [LLWL23, JXX⁺24], and video modeling [DPD⁺25, JSX⁺24].

Encouraged by their remarkable performance in language modeling, substantial efforts have been dedicated to adapting Transformers and Large Language Models (LLMs) to TSF [ZZP⁺21, LYL⁺22, WXL21, ZMW⁺22, GFQW23, CJA⁺24, PJG⁺24, JWM⁺24, JZC⁺24]. Nevertheless, empirical

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evidence consistently reveals that Transformer-based models frequently *underperform* compared to simpler, linear forecasting methods, despite their quadratic time complexity and significantly larger parameter counts [ZCZX23, TMG⁺24, ERC⁺24, LCT25]. Such findings have prompted the development of lightweight linear models and frequency-domain approaches that typically outperform Transformers on long-horizon forecasting tasks [XZX24, LQLX23, YLL⁺25, WWS⁺24, ERC⁺24]. However, a comprehensive theoretical understanding of why Transformers exhibit such limitations remains scarce.

Existing theoretical studies on Transformer for TSF mainly relied on Neural Tangent Kernel analyses or generic In-Context Learning (ICL) theory, yielding theoretical bounds often disconnected from practical relevance and failing to provide clear representational insights [KLS⁺25, CLZZ25, SGS⁺24, LIPO23, WHC⁺25]. In sharp contrast, our work uniquely addresses the core representational limitations of Transformers through a rigorous theoretical examination grounded explicitly in classical Auto-Regressive (AR) models, fundamental frameworks dominating traditional TSF [Ham20]. By adopting Linear Self-Attention (LSA), a simplified yet powerful abstraction that eliminates the Softmax function for analytical tractability [ACDS23, MHM24, ZFB24, ACS⁺24, YWS⁺24], we uncover novel and essential constraints inherent in the attention mechanism itself.

Despite AR models’ inherent linearity rendering linear methods optimal, assessing the representational gap between optimal linear models and Transformers is a highly non-trivial endeavor. Under minimal assumptions—specifically, only assuming data adheres to a stable $AR(p)$ process—we establish substantial theoretical results that clearly delineate the representational boundaries of Transformers. Our findings indicate that even optimally parameterized LSA Transformers cannot outperform classical linear predictors in terms of expected MSE. With infinitely long historical context their predictions can theoretically converge to those of linear regression if training is sufficiently good, yet even this convergence arises not from any structural advantage of LSA but from the inherent stability of time series, which collapses their representational space to that of linear models on AR processes. In contrast, for any finite context length there exists a provable strictly positive gap, which diminishes at a rate no faster than $1/n$ as the context length grows. We further analyze how predictions evolve and how errors accumulate under iterative Chain-of-Thought (CoT) inference.

Our theoretical analyses are complemented by empirical validations, providing practical insights into Transformer architectural design and clarifying their fundamental limitations in TSF contexts. Ultimately, our work calls for a reconsideration of the suitability and effectiveness of naively applying complex Transformer-based architectures to TSF. We advocate for deeper theoretical exploration to systematically unravel the foundational differences driving Transformers’ divergent performance across domains, bridging the gap between representational capability and practical efficacy.

Our primary contributions are summarized as follows:

- We show that linear self-attention is essentially a restricted/compressed representation of linear regression, so it cannot outperform linear predictors (Appendix C.1).
- We establish a strictly positive performance gap between LSA and linear predictor, and prove that this gap vanishes at a rate no faster than $1/n$ as context length increases (Appendix C.2).
- We characterize prediction behavior and error compounding rate in Chain-of-Thought inference, highlighting fundamental limitations of iterative Transformer predictions (Appendix C.3).
- We empirically corroborate our theoretical findings, offering insights into architectural implications and emphasizing the inherent representational limitations of Transformers for TSF (Appendix D).

Roadmap. In Appendix A, we review related work on positive and negative results of Transformers for time series forecasting, in-context learning theory, and representational limitations of attention. Appendix B states our problem setup and preliminary definitions. In Appendix C, we state our main theoretical contributions. In Appendix D, we describe our experimental results. Appendix E provides discussion on our perspective of TSF. Appendix F reviews classical results on time series. Appendix G analyzes the expressivity of LSA Transformers for TSF. Appendix H establishes the finite-sample gap between LSA and linear models, with detailed proofs. Appendix I extends our analysis to Chain-of-Thought rollout, characterizing collapse-to-mean and error compounding. Finally, Appendix J relaxes Gaussian assumptions and generalizes our results to linear stationary processes.

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Appendix

A Related Work

A.1 Negative Results of Transformers on TSF.

Empirical studies consistently find Transformer- and LLM-based models struggle to surpass simpler linear baselines for time series forecasting. Language modeling components add minimal value [TMG⁺24], and linear variants (NLinear, DLinear) outperform Transformers on long-horizon benchmarks [ZCZX23]. Analyses further question the utility of self-attention [KPLK24], show limited gains from scaling model size [LCT25], and motivate lightweight methods such as FITS [XZX24], RLinear [LQLX23], OLinear [YLL⁺25], TimeMixer [WWS⁺24], and CNN-based TSLANet [ERC⁺24]. Beyond forecasting, Transformers also struggle with zero-shot temporal reasoning [MTG⁺24] and anomaly detection tasks [ZY25].

Existing theoretical explanations remain limited. Kernel-based analyses attribute Transformer failures to asymmetric feature learning within a Neural Tangent Kernel regime [JGH18], but their synthetic assumptions and lack of universal lower bounds restrict their practical applicability [KLS⁺25]. Similarly, recent In-Context Learning theory for linear dynamical systems provides a data-dependent lower bound largely reflecting intrinsic noise rather than representational shortcomings [CLZZ25]. In contrast, our work studies general $AR(p)$ processes, employs distinct analytic techniques, and explicitly identifies representational constraints of Transformers relative to classical linear forecasters.

A.2 Transformers for Time Series Forecasting

Early adaptations of Transformers for time series forecasting primarily modified attention mechanisms to capture long-term dependencies efficiently. Informer introduced ProbSparse attention to mitigate quadratic complexity [ZZP⁺21], while Pyraformer employed hierarchical pyramidal attention for multi-scale modeling [LYL⁺22]. Autoformer and FEDformer further integrated domain-specific inductive biases, utilizing auto-correlation and frequency decomposition, respectively, to model seasonal-trend components explicitly [WXWL21, ZMW⁺22]. Additional variants include locality-enhanced attention [LJX⁺19], inverted architectures [LHZ⁺24], and tokenization-based representations treating sequences as textual patches [NNSK23]. A comprehensive overview is presented in [WZZ⁺23].

More recent studies leverage pretrained Large Language Models (LLMs) to transfer NLP-style capabilities to forecasting tasks. Zero-shot forecasting was initially demonstrated using pretrained LLMs without task-specific tuning [GFQW23]. Subsequent works explored specialized prompt-based strategies [CJA⁺24, PJG⁺24], reprogramming pretrained LLMs directly [JWM⁺24], and unified, dataset-agnostic training paradigms [WLK⁺24, LSY25]. Broader frameworks proposed foundational-model perspectives for time series tasks [GSC⁺24], discrete vocabulary tokenization [AST⁺24], multi-patch prediction [BJL⁺24], and generalized decoder-only architectures [DKSZ24, ZNS⁺23, LQH⁺24]. Recent surveys systematically summarize these emerging paradigms and highlight open challenges and opportunities in deploying LLMs for time series analysis [ZCGS24, LWN⁺24, LKZ⁺25, JZC⁺24].

A.3 In-Context Learning Theory

Recent work theoretically interprets in-context learning (ICL) as a Transformer forward pass implicitly performing variants of gradient descent (GD). Early studies empirically demonstrated Transformers can closely approximate ordinary-least-squares predictors [GTLV22], while subsequent constructive analyses showed one linear self-attention (LSA) layer corresponds exactly to one GD step, with the global training objective implementing a preconditioned, Bayes-optimal GD step [VONR⁺23, ASA⁺23, ACDS23, MHM24]. Further training-dynamics analyses establish gradient flow convergence of LSA to learn the class of linear models [ZFB24], provide finite-time convergence guarantees and parameter evolution for multi-head Softmax attention [HCL24, HPCY25], and identify phase transitions revealing when linear-attention mimics full Transformer behaviors [ACS⁺24, ZSL25]. Extensions include multi-step GD via chain-of-thought prompting [HWL25] and kernelized polynomial regression through gated linear units [SJA25]. Other works establish

positive approximation guarantees for ICL in dynamical and autoregressive settings but lack universal lower bounds or explicit representational constraints [LIPO23, SGS⁺24, WHC⁺25, CLZZ25].

A.4 Representational Limitations of Transformers

Despite their success, Transformers exhibit fundamental limitations in expressivity. Pure self-attention without MLPs suffers doubly exponential rank collapse with depth, severely constraining representational capacity [DCL21]. Self-attention cannot model periodic finite-state languages unless the depth or number of heads scales with input length [Hah20]. Complexity analyses show that log-precision Transformers are no more powerful than TC^0 circuits, implying provable failure on linear systems and context-free languages under standard complexity separations [MS23]. Communication-complexity arguments further reveal that Transformers cannot compose functions over sufficiently large input domains [PNP24], and their performance is task-dependent, achieving logarithmic complexity in input size for sparse averaging tasks, but requiring linear complexity for triple-detection [SHT23]. [CPW24] establish unconditional depth–width trade-offs, proving that solving sequential L -step function composition tasks over input of n tokens requires either $\Omega(L)$ layers or $n^{\Omega(1)}$ hidden dimensions. Empirically, Transformers struggle with compositional generalization [DLS⁺23] and fail to outperform RNNs in modeling Hidden Markov dynamics [HLJ24]. While chain-of-thought prompting and positional embeddings can recover arithmetic and step-wise reasoning [FZG⁺23, MBS⁺24], these function as external aids, underscoring the architecture’s inherent limitations.

B Preliminaries

Notations. We write $[n] := \{1, 2, \dots, n\}$. For $a \in \mathbb{R}^d$, let $a = (a_1, \dots, a_d)^\top$. For $X = [x_1, \dots, x_n] \in \mathbb{R}^{m \times n}$, $x_i \in \mathbb{R}^m$ is the i -th column; $X_{i,:}$ and $X_{:,j}$ denote the i -th row and j -th column; $X_{a:b,:}$ and $X_{:,c:d}$ denote row/column submatrices. $\mathbf{1}_d$, $\mathbf{0}_d$ and $\mathbf{1}_{d \times d}$, $\mathbf{0}_{d \times d}$ are all-ones/all-zeros vectors and matrices; I_d is the d -identity. $\|\cdot\|$ denotes certain norm for a vector or matrix. For symmetric $A, B \in \mathbb{R}^{d \times d}$, $A \succeq B$ ($A \succ B$) iff $A - B$ is positive semidefinite (definite). For a sequence $\{a_t\}$, $a_t \nearrow a$ means a_t increases monotonically to a . For $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$, the Kronecker product $A \otimes B \in \mathbb{R}^{mp \times nq}$ satisfies $(A \otimes B)_{(i-1)p+k, (j-1)q+\ell} := A_{i,j} B_{k,\ell}$ ($i \in [m]$, $j \in [n]$, $k \in [p]$, $\ell \in [q]$). For $X \in \mathbb{R}^{p \times p}$ symmetric, $\text{vech}(X) \in \mathbb{R}^{p(p+1)/2}$ stacks the lower triangle (incl. diagonal); for $X \in \mathbb{R}^{m \times n}$, $\text{vec}(X) \in \mathbb{R}^{mn}$ stacks columns.

B.1 Time Series

We begin by formally defining the notion of time series considered in this paper.

Definition B.1 (Time Series). A time series is a finite sequence of random variables $\{x_t\}_{t=1}^T$, indexed by discrete time $t \in \{1, \dots, T\}$. We write $x_{1:T} := (x_1, \dots, x_T)$ for the full sequence. The process is called multivariate if each $x_t \in \mathbb{R}^d$ with $d > 1$, and univariate if $d = 1$.

In this work, we primarily focus on *univariate* Auto-Regressive processes, particularly the $\text{AR}(p)$ model, a cornerstone of classical time series analysis [Ham20, BJRL15, DGH06].

Definition B.2 ($\text{AR}(p)$ Process [Ham20]). A real-valued stochastic process $\{x_i\}_{i=1}^T$ follows an autoregressive model of order p , denoted $\text{AR}(p)$, if there exist coefficients $\rho_1, \dots, \rho_p \in \mathbb{R}$ and white noise $\varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2)$ such that for all $i > 0$,

$$x_{i+1} = \sum_{j=1}^p \rho_j x_{i-j+1} + \varepsilon_{i+1},$$

with fixed initial values $\{x_{-p+1}, \dots, x_0\}$. Assuming the characteristic polynomial $1 - \rho_1 z - \dots - \rho_p z^p$ has all roots outside the unit circle, i.e. $|z| > 1$, to ensure weak stationarity, the process satisfies: (1) $\mathbb{E}[x_i] = 0$, (2) $\mathbb{E}[x_i^2] = \gamma_0$, and (3) $\mathbb{E}[x_i x_{i+k}] = \gamma_{k+1-i}$, where $\gamma_k := \mathbb{E}[x_i x_{i+k}]$ and $r_k := \gamma_k / \gamma_0$.

Further classical results—including the ordinary least squares (OLS) solution for AR models, as well as the formulation and properties of linear predictors—are deferred to Appendix F.

B.2 Transformer Architecture

For theoretical tractability, we adopt the *Linear Self-Attention (LSA)*, which omits Softmax and has been widely used in prior theoretical works [VONR⁺23, ACDS23, ZFB24, MHM24, VVSG24, GSR⁺24, GYW⁺25, SJA25, ZSL25], with growing empirical interest [KVPF20, SIS21, ACS⁺24, DG24, YWS⁺24].

Definition B.3 (Linear Self-Attention (LSA)). *Let $H \in \mathbb{R}^{(d+1) \times (m+1)}$ be the input matrix and define the causal mask $M := \begin{bmatrix} I_m & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{(m+1) \times (m+1)}$. We denote the attention weights $P, Q \in \mathbb{R}^{(d+1) \times (d+1)}$. Then the linear self-attention output is defined as*

$$\text{LSA}(H) := H + \frac{1}{m} PHM(H^\top QH) \in \mathbb{R}^{(d+1) \times (m+1)}.$$

Throughout this paper, we focus on LSA-only Transformers.

Definition B.4 (*L*-Layer LSA-Only Transformer). *Let $\text{LSA}_1, \dots, \text{LSA}_L$ be a sequence of L linear self-attention layers as defined in Definition B.3. The L -layer Transformer is defined recursively via function composition:*

$$\text{TF}(H) := \text{LSA}_L \circ \text{LSA}_{L-1} \circ \dots \circ \text{LSA}_1(H) \in \mathbb{R}^{(d+1) \times (m+1)}.$$

B.3 In-Context Time Series Forecasting

Given a univariate sequence $x_{1:n}$ of AR order p (Definition B.2), we build a Hankel matrix $H_n \in \mathbb{R}^{(p+1) \times (n-p+1)}$ (Definition B.5) whose final column is zero-padded in its last entry as a *label slot* for x_{n+1} . Setting $d = p$ and $m = n - p$, we feed H_n into the L -layer LSA-only Transformer TF (Definition B.4) and read the forecast directly from the label slot:

$$\hat{x}_{n+1} := [\text{TF}(H_n)]_{(p+1, n-p+1)} \in \mathbb{R}.$$

This representation encodes the autoregressive structure and is justified in Appendix G.3.

Definition B.5 (Hankel Matrix). *For $(x_1, \dots, x_n) \in \mathbb{R}^n$ and $p \leq n$, define*

$$H_n := \begin{bmatrix} x_1 & x_2 & \cdots & x_{n-p} & x_{n-p+1} \\ x_2 & x_3 & \cdots & x_{n-p+1} & x_{n-p+2} \\ \vdots & \vdots & & \vdots & \vdots \\ x_p & x_{p+1} & \cdots & x_{n-1} & x_n \\ x_{p+1} & x_{p+2} & \cdots & x_n & 0 \end{bmatrix} \in \mathbb{R}^{(p+1) \times (n-p+1)},$$

where each column is a sliding window of length $p+1$, with the last zero marking the prediction.

C Main Results

We organize our theoretical contributions into three parts. First, in Appendix C.1 we provide a high-level feature-space perspective: By Hankelizing the input and analyzing the induced σ -algebra, we show that one-layer linear self-attention (LSA) effectively compresses history into a restricted cubic feature class which asymptotically collapses to the last p lags, thereby anticipating a structural disadvantage relative to linear regression (LR). Building on this intuition, Appendix C.2 establishes our core result: for autoregressive (AR) and more generally linear stationary processes, the optimal one-layer LSA predictor suffers a *strict finite-sample excess risk* over LR, quantified by a positive Schur-complement gap that vanishes only asymptotically at an explicit $1/n$ rate. While stacking additional LSA layers yields monotone improvements, LR remains the fundamental benchmark that cannot be surpassed. Finally, Appendix C.3 turns to multistep forecasting: we prove that chain-of-thought (CoT) rollout, in stark contrast to its benefits in language tasks, compounds errors exponentially and collapses forecasts to the mean, with LSA uniformly dominated by LR at every horizon. All formal proofs are deferred to Appendices G, H, I and J. In contrast to prior work that mainly studies LR in ICL settings [ACDS23, ZFB24], time series settings introduce intrinsic temporal dependencies among input variables, making the analysis substantially more complex and non-trivial.

C.1 Feature-Space View

Restricted feature class. We first reparameterize P, Q in Definition B.3 to A, b to obtain the simplified form of the LSA prediction (Lemma G.3). Let $\Phi = \Phi(H_n; A, b)$ denote the one-layer LSA features induced by query-key weighting and value aggregation. The predictor admits a cubic lifting:

Lemma C.1 (Cubic lifting for one-layer LSA). *There exist coefficients $\{\beta_{j,r,k}\}$ such that*

$$\hat{x}_{n+1}^{\text{LSA}}(A, b) = \sum_{j,r,k} \beta_{j,r,k} \varphi_{j,r,k}^{(p)}(x_{1:n}), \quad \varphi_{j,r,k}^{(p)} \text{ are degree-3 monomials in } \{x_t\}.$$

Hence one-layer LSA is a linear functional over a cubic feature space $\mathcal{H}_{\text{LSA}}^{(p)}$.

Proof deferred to Appendix G. Lemma C.1 shows that the LSA readout lives in a *cubic* feature space of the raw inputs. By the L_2 -projection property of conditional expectation (orthogonality onto sub- σ -algebras), we obtain Proposition C.2: any predictor operating on Φ cannot achieve lower MSE than the optimal predictor operating on the full context $x_{1:n}$. In short, the attention-derived representation is *informationally coarser* than the raw context; adding architectural complexity does not reveal additional predictive signal beyond the last p lags, but only reweights existing information.

Proposition C.2 (Information monotonicity). $\sigma(\Phi) \subseteq \sigma(x_{1:n})$. Hence, by conditional orthogonality/Jensen,

$$\inf_f \mathbb{E}[(x_{n+1} - f(x_{1:n}))^2] \leq \inf_g \mathbb{E}[(x_{n+1} - g(\Phi))^2].$$

Proof deferred to Appendix G. Furthermore, Proposition C.3 formalizes the asymptotic picture: as the number of observed contexts $n \rightarrow \infty$, the $(p+1)$ -row Hankel design ensures access to exactly the p relevant lags; by ergodicity, empirical Hankel Gram blocks converge to their Toeplitz limits, cross-row correlations stabilize, and the cubic coordinates concentrate onto the last- p -lag subspace. Consequently, one-layer LSA *cannot outperform* LR and can at best *match it asymptotically* (Proposition G.14). See Appendix G for an optimal LSA parameter choice achieving this limit.

Proposition C.3 (Asymptotic collapse of LSA features). *As $n \rightarrow \infty$ for a stable AR(p), the coordinates $\varphi_{j,r,k}^{(p)}(x_{1:n})$ converge in L_2 to scaled copies of $\{x_{n-p+1}, \dots, x_n\}$. Thus the optimal one-layer LSA readout asymptotically reduces to a linear function of the last p lags.*

Takeaway 1: Attention is Not All You Need for TSF

Feature-Space. LSA operates on a strictly coarser σ -algebra than the raw context; it can at best reweight the last- p lags and cannot unlock signal beyond them. For time series with pronounced linear structure (e.g., AR/ARMA), this is a *fundamental representational limitation*. This aligns with empirical findings that simple linear models often outperform Transformers in TSF [ZCZX23, KPLK24, TMG⁺24].

C.2 A Strict Finite-Sample Gap (Core Result)

In this section we rigorously establish and quantitatively characterize the *fundamental representational limitation* of one-layer LSA. Our main technical device is a *Kronecker-product lifting* of the Hankel-derived features: the one-layer LSA readout can be written as

$$\hat{x}_{n+1}^{\text{LSA}} = \tilde{\eta}^\top Z, \quad Z := (\text{vech } G) \otimes x, \quad x := x_{n-p+1:n} \in \mathbb{R}^p,$$

where $G = G(x_{1:n})$ is the Hankel Gram matrix, $\text{vech}(\cdot)$ denotes half-vectorization, and $\tilde{\eta}$ is an affine reparameterization of (A, b) (see Appendix H.2). This lifts the *cubic* dependence of LSA into an ordinary *linear* regression in the lifted space. Let $Z \in \mathbb{R}^{qp}$ with $q := \dim(\text{vech } G)$. We further define $\tilde{S} := \mathbb{E}[ZZ^\top]$, $\tilde{r} := \mathbb{E}[Zx^\top]$, $\Gamma_p := \mathbb{E}[xx^\top]$, and the induced Schur complement is $\Delta_n := \Gamma_p - \tilde{r}^\top \tilde{S}^{-1} \tilde{r}$. Intuitively, Δ_n captures the component of the linear signal in the last p lags that remains *orthogonal* to the span of lifted LSA features—namely, the exact *representation gap* characterized in Theorem C.4. Moreover, we prove in Theorem C.4 that $\Delta_n \succ 0$ for any finite n , establishing a strict finite-sample gap. We then derive an explicit first-order expansion $\Delta_n = \frac{1}{n} B_p + o(1/n)$ under Gaussianity in Theorem C.5, and show in Theorems J.3 and J.5 and Lemma J.4 that both the strictness and the $1/n$ rate persist for general linear stationary processes, with the leading constant adjusted by cumulant spectra (Appendix J).

Theorem C.4 (Strict finite-sample gap: AR(p)). *For any $n \geq p$ and stable AR(p),*

$$\min_{A,b} \mathbb{E}[(\hat{x}_{n+1}^{\text{LSA}} - x_{n+1})^2] \geq \min_w \mathbb{E}[(w^\top x_{n-p+1:n} - x_{n+1})^2] + \rho^\top \Delta_n \rho, \quad \Delta_n \succ 0.$$

What this says. Even after optimizing over all one-layer LSA parameters, the *best-in-class* LSA risk is strictly larger than the *best-in-class* linear risk by the explicit quadratic form $\rho^\top \Delta_n \rho$; the gap is *structural* (positive definite), not an estimation or optimization artifact.

Why it holds. (i) The lifted loss is a strictly convex quadratic in $\tilde{\eta}$ (see Appendix H.2 and Equation (5)) with unique minimizer $\tilde{\eta}^* = \tilde{S}^{-1} \tilde{r} \rho$, yielding the class optimum $\min_{\tilde{\eta}} \mathcal{L}(\tilde{\eta}) = \sigma_\varepsilon^2 + \rho^\top \Delta_n \rho$. (ii) Under AR(p), the optimal linear predictor attains the Bayes one-step risk σ_ε^2 , so the excess risk equals $\rho^\top \Delta_n \rho$. (iii) Strictness follows from block positive definiteness of the joint covariance

$$\Sigma^\otimes := \mathbb{E} \left[\begin{pmatrix} Z \\ x \end{pmatrix} \begin{pmatrix} Z \\ x \end{pmatrix}^\top \right] = \begin{pmatrix} \tilde{S} & \tilde{r} \\ \tilde{r}^\top & \Gamma_p \end{pmatrix} \succ 0.$$

Specifically, Lemma H.6 reduces the claim to showing that the (non-lifted) joint covariance of $(\text{vech } G, x)$ is $\succ 0$; Lemma H.4 proves this via an innovation-based elimination from the newest to older indices, establishing that no nontrivial linear combination can have zero variance. The Schur-complement criterion in Lemma H.5 then yields $\Delta_n \succ 0$. All blocks admit closed forms as Hankel–Toeplitz moments up to order 4 and order 6 (from the definitions of \tilde{S} and \tilde{r} at the beginning of this section), hence Δ_n is *computable* from process moments; in the Gaussian case these moments follow from Isserlis’ theorem (Theorem H.3). A warm-up AR(1) calculation is given in Appendix H.1.

First-order gap rate under Gaussianity. We now quantify the finite- n excess risk in Theorem C.4. For zero-mean stationary Gaussian AR(p), we expand the lifted moments around their population (rank-one) limit and evaluate the Schur complement via a singular block inverse.

Theorem C.5 (Explicit $1/n$ rate: Gaussian). *For Gaussian AR(p),*

$$\Delta_n = \Gamma_p - \tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n = \frac{1}{n} B_p + o(1/n), \quad B_p \succeq 0 \text{ (generically } B_p \succ 0 \text{)}.$$

Consequently, for any fixed $\|\rho\| \geq r > 0$ there exists $c_r > 0$ such that

$$\min_{A,b} \mathbb{E}[(\hat{x}_{n+1}^{\text{LSA}} - x_{n+1})^2] \geq \min_w \mathbb{E}[(w^\top x_{n-p+1:n} - x_{n+1})^2] + \frac{c_r}{n}.$$

Proof outline. (1) *Lifted moment expansions.* Let $u = \text{vech}(\Gamma_{p+1})$. Using Isserlis formula (Theorem H.3) and Toeplitz summation (Lemma H.16), we obtain $\tilde{S}_n = (uu^\top) \otimes \Gamma_p + \frac{1}{n} C_S + o(1/n)$ and $\tilde{r}_n = u \otimes \Gamma_p + \frac{1}{n} C_r + o(1/n)$ (Lemma H.12). After block-diagonalizing along u with $P = (Q \otimes I_p)$, the leading block equals $\text{diag}(c \Gamma_p, 0)$ with $c = \|u\|^2$ and the $1/n$ corrections are $\begin{bmatrix} C_{11} & B^\top \\ B & C \end{bmatrix}$ and $\begin{bmatrix} \delta \\ d \end{bmatrix}$. Note that all parameters are defined by the time series.

(2) *Singular block inverse.* From Lemma H.13, since the orthogonal block is 0 at the limit, \hat{S}_n^{-1} has (2, 2)-block of order n . A first-order block-inverse expansion gives

$$\tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n = \Gamma_p + \frac{1}{n} B_p + o(1/n),$$

with $B_p = -\frac{1}{c} A_1 + \frac{1}{c} B^\top C^{-1} B - \frac{2}{\|u\|} B^\top C^{-1} d + d^\top C^{-1} d + \frac{2}{\|u\|} \text{Sym}(\delta)$ (Lemma H.13); hence $\Delta_n = \frac{1}{n} B_p + o(1/n)$ with $B_p := -B_p$.

Remark C.6 (Why the rate is $1/n$). *At the population limit $\tilde{S}_\infty = (uu^\top) \otimes \Gamma_p$ is rank-one along u . Finite n introduces $\Theta(1/n)$ perturbations C_S, C_r that regularize the orthogonal directions, so the Schur complement $\Gamma_p - \tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n$ is $\Theta(1/n)$. The overlap of Hankel windows is the source of these first-order terms.*

Beyond Gaussianity: strict gap and $1/n$ rate. We work under *linear stationarity* with Wold representation $x_t = \sum_{k \geq 0} \psi_k \varepsilon_{t-k}$, $\sum_k |\psi_k| < \infty$, and i.i.d. *symmetric* innovations $\{\varepsilon_t\}$ with $\mathbb{E}[\varepsilon_t] = 0$, possessing finite fourth and sixth moments. Replacing Isserlis’ theorem (Theorem H.3) by the moment–cumulant formula (Lemma J.6) preserves positive definiteness of the joint covariance, so the *strictly positive* gap still holds (Theorem J.3); furthermore, the convergence rate remains $1/n$ via the non-Gaussian expansions (Lemma J.4) culminating in the rate result (Theorem J.5).

Multi-layer LSA yields monotone improvement. Because the stacked Kronecker feature set enlarges with depth, the optimal LSA risk is monotone nonincreasing in L by projection isotonicity (Proposition H.18, using the Moore–Penrose formulation Equations (12) and (13) and the residual-covariance view Lemma H.17). Moreover, if the $(L+1)$ -st layer contributes any L_2 -nonredundant direction—equivalently $\text{Var}(P_{\mathcal{H}_L^\perp}(g^{(L)} \otimes x)) > 0$ for $\mathcal{H}_L = \text{span}\{g^{(0)} \otimes x, \dots, g^{(L-1)} \otimes x\}$ —then the Moore–Penrose Schur complement strictly decreases (Proposition H.18), yielding

$$\min_{\{b^{(\ell)}, A^{(\ell)}\}_{\ell=0}^L} \mathbb{E}[(\hat{x}_{n+1}^{(L+1)} - x_{n+1})^2] < \min_{\{b^{(\ell)}, A^{(\ell)}\}_{\ell=0}^{L-1}} \mathbb{E}[(\hat{x}_{n+1}^{(L)} - x_{n+1})^2].$$

Remark C.7. A potential misinterpretation is that we claim Transformers cannot solve or fit time series at all. This is NOT the case. Rather, our result shows that Transformers cannot outperform simple linear models beyond a certain extent. While they may be capable of solving time series tasks to some degree, their performance does not substantially exceed that of linear models.

Takeaway 2: Strictly Positive Gap between LSA and Linear Predictor

Strictness. For any finite n , one-layer LSA has a *strict* excess risk over p -lag LR equal to $\rho^\top \Delta_n \rho$ with $\Delta_n \succ 0$ (Theorem C.4).

Rate. The gap admits an explicit $1/n$ expansion with PSD leading constant B_p (generically PD) (Theorem C.5).

Robustness. Under linear stationarity with finite moments, strictness and the $1/n$ rate persist; non-Gaussianity only alters the constant via cumulants (Theorems J.3 and J.5 and Lemmas J.4 and J.6).

Depth. Stacking layers enlarges the feature span, so risk is *monotone nonincreasing* in L ; generically it *strictly* improves when the new layer adds a nonredundant direction (Proposition H.18), yet the LR baseline remains unbeatable at finite n (Equations (12) and (13)).

C.3 Chain-of-Thought Rollout: Multi-Step Collapse

Definition C.8 (Chain-of-Thought (CoT) Inference). *Given a time series (x_1, \dots, x_n) and context length p , initialize the Hankel matrix $H_n \in \mathbb{R}^{(p+1) \times (n-p+1)}$ as in Definition B.5 with the last column zero-padded. Let TF be the L -layer LSA-based Transformer in Definition B.4. For each step $t = 1, 2, \dots, T$:*

1. *Predict the next value: $\hat{x}_{n+t} := [\text{TF}(H_{n+t-1})]_{(p+1, n-p+t)}$.*
2. *Overwrite the zero in the last column of H_{n+t-1} with \hat{x}_{n+t} .*
3. *Append the column $(x_{n-p+t+1}, \dots, x_n, \hat{x}_{n+1}, \dots, \hat{x}_{n+t})^\top$ to form H_{n+t} with last entry set to 0.*

Repeating yields CoT rollouts $\hat{x}_{n+1}, \dots, \hat{x}_{n+T}$ by feeding model outputs back into the Hankel input.

Operational consequences for TSF (collapse and compounding). Under $\text{AR}(p)$, the Bayes h -step forecast equals the noise-free recursive rollout of the one-step Bayes predictor (Proposition I.1). Any stable linear CoT recursion $\hat{s}_{t+1} = A(w)\hat{s}_t$ collapses exponentially to 0 (Lemma I.2); for Bayes $w=\rho$, (Equation (14), Lemmas I.7 and I.8, and Theorem I.3):

$$\text{MSE}^*(h) = \mathbb{E}[(x_{n+h} - \hat{x}_{n+h}^*)^2] = \sigma_\varepsilon^2 \sum_{k=0}^{h-1} \psi_k^2 \nearrow \text{Var}(x_t) \quad \text{with} \quad \text{Var}(x_t) - \text{MSE}^*(h) \leq \frac{C^2 \sigma_\varepsilon^2}{1 - \beta^2} \beta^{2h}.$$

Thus, even for the optimal predictor, CoT error *compounds* to the unconditional variance at an exponential rate governed by the spectrum of $A(\rho)$.

Because conditional expectation is the L_2 projection, for any measurable $g = g(x_{1:n})$ (including any L -layer LSA CoT rollout) one has the orthogonality decomposition

$$\mathbb{E}[(x_{n+h} - g)^2] = \text{MSE}^*(h) + \mathbb{E}[(\hat{x}_{n+h}^* - g)^2] \geq \text{MSE}^*(h),$$

with strictness unless $g \equiv \hat{x}_{n+h}^*$ a.s. (Equations (16) and (17)). Since one-layer LSA already has a strict finite-sample gap at $h=1$ (Theorem C.4), equality fails generically for all h . Define the

failure horizon $H_\tau(g) := \inf\{h \geq 1 : \mathbb{E}[(x_{n+h} - g_h)^2] \geq \tau \text{Var}(x_t)\}$. Then $H_\tau(\hat{x}^{\text{LSA}}) \leq H_\tau(\hat{x}^*)$ for all $\tau \in (0, 1)$, with strict inequality on a set of τ of positive measure (Corollary I.4). In words: *LSA CoT reaches the large-error regime no later than (and generically earlier than) Bayes LR*. Quantitatively,

$$\text{Var}(x_t) - \text{MSE}^{\text{LSA}}(h) \leq \text{Var}(x_t) - \text{MSE}^*(h) \leq \frac{C^2 \sigma_\varepsilon^2}{1 - \beta^2} \beta^{2h},$$

so whenever the gap to variance remains positive, LSA’s CoT error approaches $\text{Var}(x_t)$ at least exponentially fast; if it overshoots (the left side becomes negative), Corollary I.4 still guarantees earlier threshold crossing. For AR(1), closed forms make the compounding explicit: $\text{MSE}^*(h) = \sigma^2(1 - \rho^{2h})$ with half-life $h_{1/2} = \log(1/2)/\log(\rho^2)$.

Takeaway 3: CoT Collapse in TSF

TSF. CoT rollout forms a stable linear dynamical system that *collapses to the mean* and whose error *compounds exponentially* to $\text{Var}(x_t)$; Bayes/LR is horizonwise optimal and LSA CoT is uniformly dominated at each horizon (Proposition I.1, Lemma I.2, Theorem I.3, Equation (17), and Corollary I.4).

Contrast. Notably, CoT behaves very differently in TSF compared to other domains: in language tasks, test-time scaling shows longer inference chains *improve* problem solving [LLZM24, SLXK25], and CoT can help in in-context linear regression [HWL25]; in stark contrast, in TSF, CoT leads to *rapidly compounding* forecast errors.

D Numerical Verification

D.1 Dataset and Model Configuration

Synthetic data. We generate *stable* AR(p) processes (Definition B.2) by sampling coefficient vectors (roots outside the unit circle), adding Gaussian noise, discarding a short burn-in, and retaining a long sequence. Each sequence is split into train/validation/test segments.

From long sequences to training examples. We fix a history length $n > p$. For each series $x_{1:T}$, a sliding window of length n with stride 1 defines training pairs with input history $x_{t-n+1:t}$ and target x_{t+1} . Each history is transformed into a Hankel matrix $H_n^{(t)} \in \mathbb{R}^{(p+1) \times (n-p+1)}$ (Definition B.5), which serves as the input to the LSA model.

Models. Our main model is an L -layer LSA-only Transformer TF (Definition B.4) with feature dimension $d = p$. We read prediction from the label slot: $\hat{x}_{t+1} = [\text{TF}(H_n^{(t)})]_{(p+1, n-p+1)}$. As a baseline, we fit a classical AR(p) predictor by OLS on the same training series used for LSA.

Training. All windows are shuffled and batched. Models are trained with teacher forcing using MSE loss and Adam. We sweep p , n , and L , while keeping the noise level and optimization hyperparameters fixed. Performance is reported on the held-out test split.

D.2 Evaluation

To comprehensively assess model performance in TSF, we employ two complementary inference modes for evaluation and visualization:

- **Teacher-Forcing (TF) TSF:** This method evaluates the model under idealized conditions by providing ground-truth historical values as inputs at *each* time step. It is commonly used to measure predictive accuracy and to visualize the model’s capacity to fit the true data distribution.
- **Chain-of-Thought (CoT) TSF:** This iterative inference approach simulates real-world deployment by using the model’s own past predictions as inputs for future steps. It enables the evaluation of long-horizon stability and the extent of error accumulation during rollout.

Evaluation Metrics. Let $\{x_1, x_2, \dots, x_T\}$ denote a ground-truth test time series and $\{\hat{x}_1, \hat{x}_2, \dots, \hat{x}_T\}$ the corresponding model predictions. We evaluate forecasting accuracy using the Mean Squared Error (MSE): $\text{MSE} := \frac{1}{T} \sum_{t=1}^T (x_t - \hat{x}_t)^2$. In rollouts where predictions are generated via TF or CoT, we further compute the *cumulative MSE* up to step k : $\text{CumMSE}(k) := \frac{1}{k} \sum_{t=1}^k (x_t - \hat{x}_t)^2, k \in [T]$. This captures how errors accumulate as inference progresses.

D.3 Experiments

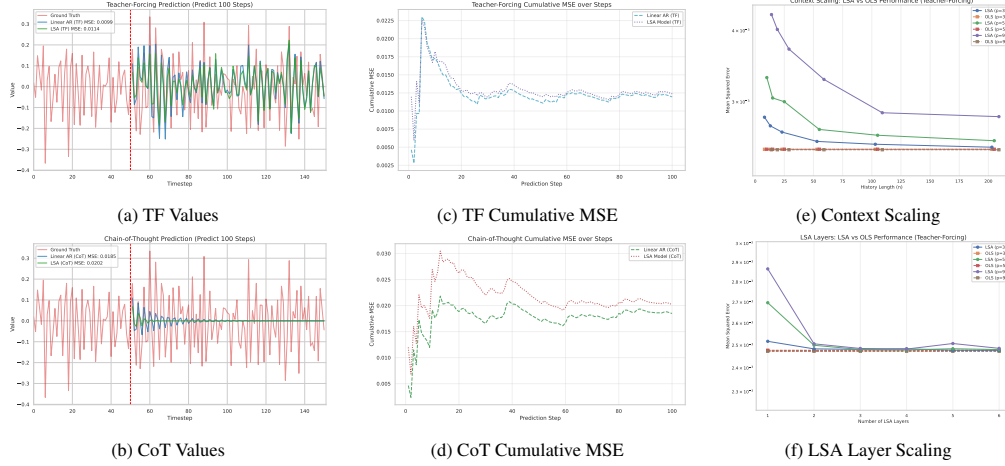


Figure 1: Experimental results. (a–b) Predictions under Teacher-Forcing (TF) and Chain-of-Thought (CoT). (c–d) Cumulative MSE for TF and CoT rollouts. (e–f) Scaling experiments varying the history length and the number of LSA layers. Overall, LSA tracks $\text{AR}(p)$ but never surpasses the OLS baseline, confirming its representational limits.

For all experiments, we adopt a common set of hyperparameters. Synthetic AR series are generated with Gaussian noise of zero mean and standard deviation $\sigma_\epsilon = 0.05$ and total length 50,000, split into training/validation/test with proportions 0.70/0.15/0.15. Models are trained for up to 150 epochs with early stopping, using a batch size of 256 and the Adam optimizer with learning rate 10^{-3} .

Teacher Forcing vs. Chain-of-Thought. We compare predictions over a 100-step horizon under Teacher-Forcing (TF) and Chain-of-Thought (CoT) rollout (Appendix D.2). Experiments use a one-layer LSA with history length $n = 20$. Figures 1 (a–b) and (c–d) report the predicted trajectories and cumulative MSEs. Under TF, both LSA and OLS follow the ground-truth $\text{AR}(p)$ process with only minor MSE differences, indicating that LSA can fit the data but never surpasses the linear baseline. Under CoT rollout, however, errors compound over time: both LSA and OLS collapse toward the mean, with LSA collapsing earlier, consistent with our theoretical predictions in Appendix C.3.

Context and Layers Scaling. We examine the effect of varying the history length n and the number of LSA layers L . For context scaling, we sweep $n = p + \{5, 10, 20, 50, 100, 200\}$ with a single LSA layer. For layer scaling, we vary $L \in \{1, 2, 3, 4, 5, 6\}$ while fixing $n = 100$. Figures 1 (e–f) report the Teacher-Forcing MSE on the test series. Increasing n improves LSA performance but never closes the gap to the linear baseline. Similarly, adding layers yields improvement saturating at the OLS level rather than surpassing it. Together, these findings validate our theory in Appendix C.2.

E Discussion

Architectural Considerations. Beyond LSA, several components may influence Transformer performance. The Softmax in standard attention may enhance expressivity by exponentiating inputs, possibly expanding the space and approximating an infinite sum to capture richer dependencies. Given the limitations of single-head LSA, simply aggregating multiple heads over the same data source is unlikely to improve expressivity; however, allocating different heads to distinct modalities may

offer benefits through data fusion. Additionally, the role of feedforward MLP layers deserves closer scrutiny. Although not the focus of our analysis, prior work [ZCZX23, TMG⁺24, KPLK24] suggests that MLPs play as key contributors in time series tasks—potentially explaining the performance of LLMs in TSF. We leave these directions to future work.

Difference Between Language and Time Series. Attention serves as a learned compression mechanism, essential in language modeling where meaning depends on long-range, abstract dependencies [DRD⁺24, Sut23, GFRW24, HZSH24]. In contrast, time series with low-order dynamics (e.g., $AR(p)$) hinge on local, position-specific patterns, where such compression can obscure predictive signals. Because attention applies fixed contextual weights, it often fails to capture these direct dependencies, explaining the locality-agnostic behavior noted in [LJX⁺19]. When compression is misaligned with the data-generating process, classical models typically outperform attention.

Other Data Distributions. Although our analysis focuses on AR processes, similar considerations apply more broadly. The difficulty for attention arises from its misalignment in capturing input dependencies, as seen in $AR(p)$. We further discuss Moving Average (MA) processes and, more generally, ARMA models in Appendix J.

Multivariate Time Series. In the case of uncorrelated multivariate time series, each dimension evolves independently, reducing training to separate LSA models. This eliminates the opportunity to exploit cross-variable dependencies and limits the potential of learning shared structure. Consequently, pretraining on a collection of uncorrelated time series may fail to produce useful shared representations. For the correlated case, one could impose structural assumptions on inter-variable dependencies to enable tractable analysis. We leave the investigation of such multivariate models, such as Vector Auto-Regression (VAR) [Ham20], to future work.

Optimization Dynamics. While our analysis primarily addresses representational limitations of attention mechanisms, future work could explore optimization dynamics and training difficulties of Transformers for time series forecasting. Understanding these issues might yield complementary insights into observed empirical shortcomings.

Real-World Complexities. Real-world forecasting tasks include many complexities not modeled in this study, such as data randomness, intricate temporal dependencies, training instability, noisy signals, and external factors like market sentiment [LWN⁺24, LKZ⁺25]. Exploring these practical challenges could help bridge theoretical findings with real-world performance.

Architectural and Framework Varieties. Our framework intentionally abstracts away practical components such as Rotary Position Embeddings (RoPE) [SAL⁺24] and Mixture-of-Experts (MoE) [FZS22]. Future work may assess whether these enhancements alleviate the representational limitations we identify. State Space Models like Mamba [GD24, DG24] also present a promising alternative for time series forecasting [WKF⁺25]. Beyond architectural changes, generative modeling paradigms such as diffusion models [HJA20] and flow matching [LCBH⁺23] offer alternative approaches for time series [TSSE21, YQ24, HWW⁺24, LYLH24, FWX⁺24], potentially overcoming the limitations of Transformer-based Next-Token Prediction objectives.

F Time Series Fundamentals

We first recall classical results for stationary autoregressive (AR) processes, which form the theoretical backbone for our later analysis. These results connect population-level covariances to model coefficients, show how consistent estimates can be obtained from finite data, and establish a natural linear performance baseline.

Definition F.1 (Yule–Walker Equations [Ham20]). *Let $\{x_i\}_{i=1}^T$ follow a stationary $AR(p)$ process as in Definition B.2. Define the Toeplitz autocovariance matrix $\Gamma_p \in \mathbb{R}^{p \times p}$ as*

$$\Gamma_p := \begin{pmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_{p-1} \\ \gamma_1 & \gamma_0 & \cdots & \gamma_{p-2} \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_{p-1} & \gamma_{p-2} & \cdots & \gamma_0 \end{pmatrix}, \quad \gamma := \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_p \end{pmatrix}.$$

Then the AR coefficient vector $\rho := (\rho_1, \dots, \rho_p)^\top$ satisfies the Yule–Walker system:

$$\Gamma_p \rho = \gamma.$$

This moment-matching condition links the autocovariance structure to the autoregressive coefficients.

Theorem F.2 (OLS Consistency for AR(p) Estimation [Ham20]). *Let $\{x_i\}_{i=1}^T$ be generated by an AR(p) process as in Definition B.2. Let $\hat{\rho}_n := (X^\top X)^{-1} X^\top y$ be the ordinary least squares estimator obtained from*

$$y := (x_{p+1}, \dots, x_n)^\top, \quad X := \begin{pmatrix} x_p & x_{p-1} & \cdots & x_1 \\ x_{p+1} & x_p & \cdots & x_2 \\ \vdots & \vdots & \ddots & \vdots \\ x_{n-1} & x_{n-2} & \cdots & x_{n-p} \end{pmatrix}.$$

Then, as $n \rightarrow \infty$,

$$\hat{\rho}_n \xrightarrow{\text{a.s.}} \rho.$$

Hence, in the large-sample limit, OLS recovers the Bayes-optimal linear predictor in mean squared error.

Theorem F.3 (Linear Baseline under AR(p) Dynamics). *Let $\{x_i\}_{i=1}^T$ be generated by an AR(p) process as in Definition B.2. Fix a context window $x_{1:n} \in \mathbb{R}^n$ with $n \geq p$. For any linear predictor $\hat{x}_{n+1}^{\text{LR}} = w^\top x_{1:n}$ we have*

$$\min_{w \in \mathbb{R}^n} \mathbb{E}[(w^\top x_{1:n} - x_{n+1})^2] < \text{Var}(x_{n+1}),$$

where the expectation is over the stationary joint distribution of (x_1, \dots, x_{n+1}) .

Proof. By Definition B.2, $\mathbb{E}[x_i] = 0$ and the noise variance is σ^2 . The Bayes-optimal (and hence optimal linear) predictor is

$$\hat{x}_{n+1}^{\text{LR}} = \mathbb{E}[x_{n+1} \mid x_{1:n}] = \sum_{j=1}^p \rho_j x_{n-j+1}.$$

Its mean squared error is

$$\mathbb{E}[(\hat{x}_{n+1}^{\text{LR}} - x_{n+1})^2] = \sigma^2 < \sigma^2 + \text{Var}(x_n) = \text{Var}(x_{n+1}),$$

which is strictly below the variance baseline. □

G Transformers Expressivity for TSF

G.1 Fundamentals of Linear Self-Attention

We work with Hankelized inputs for time-series forecasting. For context length p and total length $n \geq p$, define the Hankel matrix

$$H = [x^{(1)} \ x^{(2)} \ \dots \ x^{(n-p+1)}] \in \mathbb{R}^{(p+1) \times (n-p+1)},$$

where each $x^{(i)} \in \mathbb{R}^{p+1}$ stacks a length- p window and a $(p+1)$ -st *label slot*; we reserve the last column $x^{(n-p+1)}$ as the prediction token (see Definition B.5 for construction details).

Definition G.1 (Linear Self-Attention (single layer)). *Let $P, Q \in \mathbb{R}^{(p+1) \times (p+1)}$ be trainable. Define*

$$S := H^\top Q H \in \mathbb{R}^{(n-p+1) \times (n-p+1)}, \quad M := \text{diag}(I_{n-p}, 0) \in \mathbb{R}^{(n-p+1) \times (n-p+1)}.$$

The one-layer LSA update is

$$\text{LSA}(H) := H + \frac{1}{n} P (H M S) \in \mathbb{R}^{(p+1) \times (n-p+1)}, \quad (1)$$

where M masks the prediction token to avoid self-use during the update.

The multi-layer variant is defined by composing L residual bilinear updates.

Definition G.2 (L -layer LSA Transformer). *For parameters $\{P_\ell, Q_\ell\}_{\ell=1}^L$, define each layer as*

$$\text{LSA}_\ell(H) := H + \frac{1}{n} P_\ell (H M (H^\top Q_\ell H)),$$

and the overall L -layer LSA Transformer as

$$\text{TF}(H) := \text{LSA}_L \circ \dots \circ \text{LSA}_1(H).$$

We now formalize the readout at the prediction slot for a single LSA layer, which will later serve as the basic building block in our theoretical analysis.

Lemma G.3 (Closed-form readout of one-layer LSA on Hankel input [ACDS23]). *Following the construction in Definition B.5 and Definition G.1, the final column of H is the prediction token,*

$$x^{(n-p+1)} = \begin{bmatrix} x_{n-p+1:n} \\ 0 \end{bmatrix}, \quad x_{n-p+1:n} \in \mathbb{R}^p.$$

Suppose

$$P = \begin{bmatrix} \mathbf{0}_{p \times (p+1)} \\ b^\top \end{bmatrix}, \quad Q = \begin{bmatrix} A & \mathbf{0}_{(p+1) \times 1} \end{bmatrix},$$

with $b \in \mathbb{R}^{p+1}$ and $A \in \mathbb{R}^{(p+1) \times p}$. Then the prediction-slot entry satisfies

$$[\text{LSA}(H)]_{p+1, n-p+1} = b^\top G_n A x_{n-p+1:n},$$

where we define the empirical Gram matrix

$$G_n := \frac{1}{n} \sum_{i=1}^{n-p} x^{(i)} x^{(i)\top}.$$

Proof. Let $S = H^\top Q H$. Since the last column of M is zero,

$$H M = [x^{(1)} \ \dots \ x^{(n-p)} \ 0].$$

Because $[H]_{p+1, n-p+1} = 0$ and $e_{p+1}^\top P = b^\top$,

$$[\text{LSA}(H)]_{p+1, n-p+1} = \frac{1}{n} b^\top (H M S) e_{n-p+1} = \frac{1}{n} \sum_{j=1}^{n-p} b^\top x^{(j)} S_{j, n-p+1}.$$

For $j \leq n-p$,

$$S_{j, n-p+1} = x^{(j)\top} Q x^{(n-p+1)} = x^{(j)\top} A x_{n-p+1:n},$$

which gives the stated expression. \square

G.2 Function Space Constraints of Linear Self-Attention

In this subsection we take a function-space perspective on linear self-attention. Rather than analyzing specific computations, we characterize the class of functions that a one-layer LSA readout can realize on Hankelized inputs. This higher-level view makes explicit that LSA predictions are confined to a restricted polynomial feature space, and thus—despite the nontrivial attention mechanism—cannot achieve fundamentally lower risk than classical linear regression on $\text{AR}(p)$ processes.

Lemma G.4 (Doob–Dynkin [Kal06]). *Let $f : \Omega \rightarrow S$ and $g : \Omega \rightarrow T$ be measurable mappings between measurable spaces. Then f is $\sigma(g)$ -measurable if and only if there exists a measurable $h : T \rightarrow S$ such that $f = h \circ g$.*

Theorem G.5 (Projection Monotonicity in L^2). *Let H be a Hilbert space and $M_2 \subseteq M_1 \subseteq H$ be closed subspaces. For any $Z \in H$, letting P_{M_i} denote the orthogonal projection onto M_i , we have*

$$\|Z - P_{M_1} Z\| \leq \|Z - P_{M_2} Z\|.$$

Functional form of the one-layer readout. Let $H = [x^{(1)} \dots x^{(n-p+1)}] \in \mathbb{R}^{(p+1) \times (n-p+1)}$ be the Hankel matrix from Definition B.5. Following Definition G.1, the one-layer LSA update is

$$\text{LSA}(H) = H + \frac{1}{n} P(H M (H^\top Q H)).$$

Following Definition B.5, the final column of H is the prediction token,

$$x^{(n-p+1)} = \begin{bmatrix} x_{n-p+1:n} \\ 0 \end{bmatrix}, \quad x_{n-p+1:n} \in \mathbb{R}^p.$$

By Lemma G.3, for suitable trainable P, Q ,

$$[\text{LSA}(H)]_{p+1, n-p+1} = b^\top G_n A x_{n-p+1:n}, \quad G_n := \frac{1}{n} \sum_{i=1}^{n-p} x^{(i)} x^{(i)\top}.$$

Definition G.6 (LSA feature space). *For $j, r \in [p+1]$ and $k \in [p]$, define the cubic coordinates*

$$\phi_{j,r,k}^{(p)}(x_{1:n}) := \frac{1}{n} \sum_{i=1}^{n-p} x_{i+j-1} x_{i+r-1} x_{i-p+k}.$$

Collect them into the feature map

$$\Phi^{(p)}(x_{1:n}) := (\phi_{j,r,k}^{(p)}(x_{1:n}))_{j,r \in [p+1], k \in [p]} \in \mathbb{R}^m, \quad m = p(p+1)^2,$$

and define the linear self-attention feature space

$$\mathcal{H}_{\text{LSA}}^{(p)} := \text{span}\left\{\phi_{j,r,k}^{(p)}(\cdot) : j, r \in [p+1], k \in [p]\right\}.$$

Since each coordinate is a finite sum of degree-3 monomials, $\Phi^{(p)}$ is continuous.

Theorem G.7 (Representation of one-layer LSA readout). *There exist coefficients $\{\beta_{j,r,k}\}$, depending on the trainable parameters in P, Q , such that*

$$\hat{x}_{n+1} = [\text{LSA}(H)]_{p+1, n-p+1} = \sum_{j=1}^{p+1} \sum_{r=1}^{p+1} \sum_{k=1}^p \beta_{j,r,k} \phi_{j,r,k}^{(p)}(x_{1:n}) \in \mathcal{H}_{\text{LSA}}^{(p)}.$$

Proof. By Lemma G.3, for suitable trainable P, Q ,

$$[\text{LSA}(H)]_{p+1, n-p+1} = b^\top G_n A x_{n-p+1:n}, \quad G_n := \frac{1}{n} \sum_{i=1}^{n-p} x^{(i)} x^{(i)\top}.$$

Expanding the product gives

$$b^\top G_n A x_{n-p+1:n} = \sum_{j=1}^{p+1} \sum_{r=1}^{p+1} \sum_{k=1}^p (b_j A_{r,k}) \phi_{j,r,k}^{(p)}(x_{1:n}),$$

where we define $\beta_{j,r,k} := b_j A_{r,k}$. This matches the claimed representation. \square

Theorem G.8 (Risk monotonicity under LSA features). *Let $(x_{1:n}, x_{n+1})$ be jointly defined random variables. Under squared loss,*

$$\inf_f \mathbb{E} \left[(x_{n+1} - f(x_{1:n}))^2 \right] \leq \inf_g \mathbb{E} \left[(x_{n+1} - g(\Phi^{(p)}(x_{1:n})))^2 \right].$$

Equality holds if and only if $x_{n+1} \perp\!\!\!\perp x_{1:n} \mid \Phi^{(p)}(x_{1:n})$.

Proof. By optimality of conditional expectations, the minimizers are $\mathbb{E}[x_{n+1} \mid x_{1:n}]$ and $\mathbb{E}[x_{n+1} \mid \Phi^{(p)}(x_{1:n})]$. Since $\Phi^{(p)}$ is a deterministic function of $x_{1:n}$, Doob–Dynkin (Lemma G.4) gives $\sigma(\Phi^{(p)}(x_{1:n})) \subseteq \sigma(x_{1:n})$. Conditional expectation is the L^2 projection, so Theorem G.5 yields the inequality; the equality condition is standard. \square

Theorem G.9 (Single-layer LSA cannot beat the linear predictor under AR(p)). *Suppose $\{x_t\}$ follows a stationary AR(p) process with context $x_{1:n}$ and $n \geq p$. Let $\hat{x}_{n+1}^{\text{LSA}}$ denote any one-layer LSA readout as in Theorem G.7. Then*

$$\inf \mathbb{E} \left[(\hat{x}_{n+1}^{\text{LSA}} - x_{n+1})^2 \right] \geq \inf_{w \in \mathbb{R}^n} \mathbb{E} \left[(w^\top x_{1:n} - x_{n+1})^2 \right].$$

Proof. By Theorem G.7, $\hat{x}_{n+1}^{\text{LSA}}$ is a measurable function of $\Phi^{(p)}(x_{1:n})$, hence its best risk is at least that of the Bayes predictor given $\Phi^{(p)}(x_{1:n})$; Theorem G.8 then lower-bounds this by the Bayes risk given $x_{1:n}$. Under AR(p), $\mathbb{E}[x_{n+1} \mid x_{1:n}]$ is linear in $x_{1:n}$, so the Bayes risk equals the optimal linear risk. Hence the claim. \square

G.3 Nested Transformer Feature Spaces and Risk Monotonicity in Time Series Prediction

We take a function-space perspective: with Hankel inputs and a masked label slot, the one-layer LSA readout operates in a restricted feature class. As the sequence length grows, these features collapse to scaled copies of the last p lags, which clarifies both our Hankel design ($p+1$ rows) and why one-layer LSA cannot fundamentally beat linear regression on AR(p).

Setup. Throughout this subsection we work under the AR(p) model in Definition B.2, the Hankel construction in Definition B.5, the one-layer LSA update in Definition G.1, and the cubic coordinates in Definition G.6. Let M be the mask from Definition G.1.

Theorem G.10 (Ergodic Theorem, Birkhoff [Kal06]). *Let ξ be a random element in a measurable space S with distribution μ , and let $T : S \rightarrow S$ be a μ -preserving transformation with invariant σ -field \mathcal{I} . Then for any measurable function $f \geq 0$ on S , we have*

$$\frac{1}{n} \sum_{k=0}^{n-1} f(T^k \xi) \xrightarrow{\text{a.s.}} \mathbb{E}[f(\xi) \mid \mathcal{I}],$$

where the convergence is almost surely.

Lemma G.11 (Asymptotic feature collapse). *Define the normalized masked Hankel Gram*

$$G_n := \frac{1}{n} H M H^\top.$$

Then, entrywise, $G_n \xrightarrow{\text{a.s.}} \Gamma_{p+1}$, where $[\Gamma_{p+1}]_{ij} = \gamma_{|i-j|}$ and $\gamma_h = \mathbb{E}[x_t x_{t+h}]$. Moreover, for the cubic coordinates $\phi_{j,r,k}^{(p)}$ in Definition G.6,

$$\phi_{j,r,k}^{(p)}(x_{1:n}) \xrightarrow{\text{a.s.}} \gamma_{|j-r|} x_{n-p+k}, \quad j, r \in [p+1], \quad k \in [p].$$

Hence,

$$\text{span}\{\phi_{j,r,k}^{(p)}(x_{1:n})\} \xrightarrow{\text{a.s.}} \text{span}\{x_{n-p+1}, \dots, x_n\}.$$

Proof. Each entry of G_n is a time average of $x_{i+a-1} x_{i+b-1}$; by Birkhoff’s ergodic theorem (Theorem G.10), $G_n \rightarrow \Gamma_{p+1}$ almost surely. For $\phi_{j,r,k}^{(p)}$, factor out x_{n-p+k} and apply the same theorem to $\frac{1}{n} \sum_i x_{i+j-1} x_{i+r-1}$. \square

Corollary G.12 (Nested spaces). *Let $\tilde{\mathcal{H}}_{\text{LSA}}^{(p)} := \text{span}\{x_{n-p+1}, \dots, x_n\}$. Then $\tilde{\mathcal{H}}_{\text{LSA}}^{(p)} \subseteq \tilde{\mathcal{H}}_{\text{LSA}}^{(p+1)}$ for all p .*

Theorem G.13 (Risk plateau on AR(p)). *Under AR(p), the Bayes predictor is linear in the last p lags: $x_{n+1} = \sum_{j=1}^p \rho_j x_{n-j+1} + \varepsilon_{n+1}$ with $\mathbb{E}[\varepsilon_{n+1} \mid x_{1:n}] = 0$. By Lemma G.11 and Corollary G.12, any one-layer LSA based on Hankel features operates (as $n \rightarrow \infty$) on $\text{span}\{x_{n-p+1}, \dots, x_n\}$. Therefore, the minimal achievable MSE equals the linear Bayes risk σ_ε^2 and does not decrease for $q \geq p$:*

$$\inf_f \mathbb{E} \left[(x_{n+1} - f(\text{LSA features of order } q))^2 \right] = \sigma_\varepsilon^2, \quad \forall q \geq p.$$

Proposition G.14 (Asymptotic exact recovery: a constructive parameter choice). *Let the one-layer readout at the prediction slot be written as in Lemma G.3:*

$$[\text{LSA}(H)]_{p+1, n-p+1} = b^\top G_n A x_{n-p+1:n},$$

with $b \in \mathbb{R}^{p+1}$ and $A \in \mathbb{R}^{(p+1) \times p}$. Define

$$b^* := (0, \dots, 0, 1)^\top \in \mathbb{R}^{p+1}, \quad A^* := \begin{bmatrix} J \Gamma_p^{-1} \\ \mathbf{0}_{1 \times p} \end{bmatrix} \in \mathbb{R}^{(p+1) \times p},$$

where $J \in \mathbb{R}^{p \times p}$ is the anti-diagonal permutation (reversal) matrix and Γ_p is the $p \times p$ autocovariance Toeplitz matrix. Then, as $n \rightarrow \infty$,

$$b^{*\top} G_n A^* x_{n-p+1:n} \xrightarrow{\text{a.s.}} \rho^\top x_{n-p+1:n},$$

i.e., the one-layer LSA readout exactly recovers the Bayes-optimal linear predictor in the limit.

Proof. By Lemma G.11, $G_n \rightarrow \Gamma_{p+1}$. Since $b^{*\top} \Gamma_{p+1} = [\gamma_p, \dots, \gamma_1, \gamma_0]$, we get

$$b^{*\top} \Gamma_{p+1} A^* = [\gamma_p, \dots, \gamma_1] J \Gamma_p^{-1} = [\gamma_1, \dots, \gamma_p] \Gamma_p^{-1} = \rho^\top,$$

using the Yule–Walker relation $\rho = \Gamma_p^{-1} \gamma$ with $\gamma = (\gamma_1, \dots, \gamma_p)^\top$. \square

Why exactly $p+1$ Hankel rows. The first p rows are necessary to capture the true p lags of the AR(p) process, while the $(p+1)$ -st row serves as the masked prediction slot. With fewer than $p+1$ rows, the model cannot access all p relevant lags. With more than $p+1$ rows, the extra rows are asymptotically redundant, since the optimal predictor ultimately depends only on the last p lags.

H Closed-Form Gap Characterization between LSA and Linear Models

H.1 Warm Up via AR(1)

Warm-up, not global optimum. Motivated by the asymptotic constructive choice in Proposition G.14 (where b has the last entry 1 and the last row of A is 0), we study the univariate AR(1) case and *restrict* (b, A) to the one-dimensional ray induced by that limiting structure. This gives a computable warm start that illustrates how Isserlis' theorem (Theorem H.3) enters the calculation; it is not the global optimum over all (b, A) , but it tends to linear regression as $n \rightarrow \infty$.

Proposition H.1 (AR(1) warm start along the asymptotic ray). *Let $\{x_t\}$ be the stationary Gaussian AR(1) process of Definition B.2:*

$$x_t = \rho x_{t-1} + \varepsilon_t, \quad |\rho| < 1, \quad \varepsilon_t \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2),$$

and set $\sigma^2 := \sigma_\varepsilon^2 / (1 - \rho^2) = \text{var}(x_t)$. For context $p = 1$ and $n \geq 3$, let H_n be the Hankel matrix (Definition B.5) with mask $M = \text{diag}(I_{n-1}, 0)$ and define the normalized Gram

$$G_n := \frac{1}{n} H_n M H_n^\top = \frac{1}{n} \sum_{i=1}^{n-1} \begin{pmatrix} x_i^2 & x_i x_{i+1} \\ x_i x_{i+1} & x_{i+1}^2 \end{pmatrix}.$$

Let $S_n := \frac{1}{n} \sum_{i=1}^{n-1} x_i x_{i+1}$. Restrict (b, A) to

$$b = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad A = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}, \quad \alpha \in \mathbb{R},$$

so the one-layer LSA readout at the prediction slot is

$$\hat{y}_n(\alpha) = (b^\top G_n A) x_n = \alpha S_n x_n.$$

Consider the surrogate loss against the AR(1) linear term:

$$\mathcal{L}(\alpha) = \mathbb{E}[(\hat{y}_n(\alpha) - \rho x_n)^2] = \mathbb{E}[x_n^2 (\alpha S_n - \rho)^2] = \alpha^2 D_n - 2\alpha \rho N_n + \rho^2 \sigma^2.$$

Define the geometric sums (for $m \geq 1$)

$$K_m := \sum_{k=1}^m \rho^{2k} = \frac{\rho^2(1 - \rho^{2m})}{1 - \rho^2}, \quad H_m := \sum_{k=1}^m k \rho^{2k} = \frac{\rho^2(1 - (m+1)\rho^{2m} + m\rho^{2(m+1)})}{(1 - \rho^2)^2}.$$

Then, with $\Gamma_k := \text{Cov}(x_t, x_{t+k}) = \sigma^2 \rho^{|k|}$,

$$N_n := \mathbb{E}[x_n^2 S_n] = \frac{\sigma^4}{n} \left[(n-1)\rho + \frac{2}{\rho} K_{n-1} \right], \quad (2)$$

$$D_n := \mathbb{E}[x_n^2 S_n^2] = \frac{\sigma^6}{n^2} \left[(n-1)n\rho^2 + (n-1) + (4(n-1) - 2)K_{n-1} \right. \\ \left. + (4(n-1) + 2)K_{n-2} + 8H_{n-1} + 4H_{n-2} \right]. \quad (3)$$

Consequently the unique minimizer along this ray and its value are

$$\alpha^* = \frac{\rho N_n}{D_n}, \quad \min_{\alpha} \mathcal{L}(\alpha) = \rho^2 \sigma^2 - \frac{\rho^2 N_n^2}{D_n}.$$

Equivalently,

$$\min_{\alpha} \mathbb{E}[(\hat{x}_{n+1}^{\text{LSA}} - x_{n+1})^2] = \sigma_\varepsilon^2 + \rho^2 \sigma^2 - \frac{\rho^2 N_n^2}{D_n},$$

and, by the law of large numbers and dominated convergence,

$$\alpha^* \xrightarrow{n \rightarrow \infty} \frac{1}{\sigma^2}, \quad \min_{\alpha} \mathcal{L}(\alpha) \xrightarrow{n \rightarrow \infty} 0,$$

i.e., this warm start tends to the linear-regression limit.

Proof. **Step 1: N_n —pairwise expansion (4th order).**

$$N_n = \frac{1}{n} \sum_{i=1}^{n-1} \mathbb{E}[x_n^2 x_i x_{i+1}].$$

For the zero-mean Gaussian quadruple (x_n, x_n, x_i, x_{i+1}) , by Isserlis (Theorem H.3) the three pairings give

$$\begin{aligned} (x_n, x_n)(x_i, x_{i+1}) &\Rightarrow \Gamma_0 \Gamma_1 = \sigma^4 \rho, \\ (x_n, x_i)(x_n, x_{i+1}) &\Rightarrow \Gamma_{n-i} \Gamma_{n-i-1} = \sigma^4 \rho^{2n-2i-1}, \\ (x_n, x_{i+1})(x_n, x_i) &\Rightarrow \Gamma_{n-i-1} \Gamma_{n-i} = \sigma^4 \rho^{2n-2i-1}. \end{aligned}$$

Hence $\mathbb{E}[x_n^2 x_i x_{i+1}] = \sigma^4 (\rho + 2\rho^{2n-2i-1})$, and summing over i yields (2).

Step 2: D_n —pairwise expansion (6th order).

$$D_n = \frac{1}{n^2} \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} \mathbb{E}[x_n^2 x_i x_{i+1} x_j x_{j+1}]$$

splits into diagonal ($i = j$) and off-diagonal ($i < j$) parts.

Diagonal $i = j$. With $X := x_n$, $Y := x_i$, $Z := x_{i+1}$,

$$\mathbb{E}[X^2 Y^2 Z^2] = \Gamma_0^3 + 2\Gamma_{XY}^2 \Gamma_0 + 2\Gamma_{XZ}^2 \Gamma_0 + 2\Gamma_{YZ}^2 \Gamma_0 + 8\Gamma_{XY} \Gamma_{XZ} \Gamma_{YZ}.$$

Substituting $\Gamma_0 = \sigma^2$, $\Gamma_{XY} = \sigma^2 \rho^{n-i}$, $\Gamma_{XZ} = \sigma^2 \rho^{n-i-1}$, $\Gamma_{YZ} = \sigma^2 \rho$ and summing over $i = 1, \dots, n-1$ gives the diagonal contribution

$$\sigma^6 \left((n-1) + 2\rho^2(n-1) + 2 \sum_{k=1}^{n-2} \rho^{2k} + 10 \sum_{k=1}^{n-1} \rho^{2k} \right) = \sigma^6 \left((n-1) + 2\rho^2(n-1) + 2K_{n-2} + 10K_{n-1} \right).$$

Off-diagonal $i < j$. Let $Y_1 := x_i$, $Y_2 := x_{i+1}$, $Z_1 := x_j$, $Z_2 := x_{j+1}$. Grouping the 15 pairings by how the two copies of x_n are paired gives the per- (i, j) contributions listed below (the factor “ $\times 2$ ” indicates the symmetric counterpart):

$(x_n, x_n)(Y_1, Y_2)(Z_1, Z_2)$	$\Rightarrow \sigma^6 \rho^2$
$(x_n, x_n)(Y_1, Z_1)(Y_2, Z_2)$	$\Rightarrow \sigma^6 \rho^{2(j-i)}$
$(x_n, x_n)(Y_1, Z_2)(Y_2, Z_1)$	$\Rightarrow \sigma^6 \rho^{2(j-i)}$
$\{(x_n, Y_1), (x_n, Y_2)\}, (Z_1, Z_2) (\times 2)$	$\Rightarrow 2\sigma^6 \rho^{2(n-i)}$
$\{(x_n, Z_1), (x_n, Z_2)\}, (Y_1, Y_2) (\times 2)$	$\Rightarrow 2\sigma^6 \rho^{2(n-j)}$
$\{(x_n, Y_1), (x_n, Z_1)\}, (Y_2, Z_2) (\times 2)$	$\Rightarrow 2\sigma^6 \rho^{2(n-i)}$
$\{(x_n, Y_1), (x_n, Z_2)\}, (Y_2, Z_1) (\times 2)$	$\Rightarrow 2\sigma^6 \rho^{2(n-i)}$
$\{(x_n, Y_2), (x_n, Z_1)\}, (Y_1, Z_2) (\times 2)$	$\Rightarrow 2\sigma^6 \rho^{2(n-i-1)}$
$\{(x_n, Y_2), (x_n, Z_2)\}, (Y_1, Z_1) (\times 2)$	$\Rightarrow 2\sigma^6 \rho^{2(n-i-1)}$

Summing over $1 \leq i < j \leq n-1$ and reindexing,

$$\begin{aligned} &\sum_{1 \leq i < j \leq n-1} \mathbb{E}[x_n^2 x_i x_{i+1} x_j x_{j+1}] \\ &= \sigma^6 \left(\binom{n-1}{2} \rho^2 + 2 \sum_{k=1}^{n-1} (n-1-k) \rho^{2k} + 6 \sum_{i=1}^{n-1} (n-1-i) \rho^{2(n-i)} \right. \\ &\quad \left. + 4 \sum_{i=1}^{n-1} (n-1-i) \rho^{2(n-1-i)} + 2 \sum_{k=1}^{n-2} (n-1-k) \rho^{2k} \right) \\ &= \sigma^6 \left(\binom{n-1}{2} \rho^2 + (2n-8)K_{n-1} + 4H_{n-1} + 2(n-1)K_{n-2} + 2H_{n-2} \right). \end{aligned}$$

Finally, we obtain the final expression of D_n

$$\begin{aligned}
D_n &= \frac{1}{n^2} \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} \mathbb{E}[x_n^2 x_i x_{i+1} x_j x_{j+1}] \\
&= \frac{1}{n^2} \sum_{1 \leq i=j \leq n-1} \mathbb{E}[x_n^2 x_i x_{i+1} x_j x_{j+1}] + \frac{2}{n^2} \sum_{1 \leq i < j \leq n-1} \mathbb{E}[x_n^2 x_i x_{i+1} x_j x_{j+1}] \\
&= \frac{\sigma^6}{n^2} \left((n-1) + 2\rho^2(n-1) + 2K_{n-2} + 10K_{n-1} \right) \\
&\quad + \frac{2\sigma^6}{n^2} \left(\binom{n-1}{2} \rho^2 + (2n-8)K_{n-1} + 4H_{n-1} + 2(n-1)K_{n-2} + 2H_{n-2} \right). \\
&= \frac{\sigma^6}{n^2} \left[(n-1)n\rho^2 + (n-1) + (4(n-1)-2)K_{n-1} + (4(n-1)+2)K_{n-2} + 8H_{n-1} + 4H_{n-2} \right].
\end{aligned}$$

Adding the diagonal part and multiplying by $1/n^2$ yields (3).

Step 3: Limit and conclusion. Since $D_n > 0$, \mathcal{L} is strictly convex, so the minimizer and value follow. As $S_n \rightarrow \mathbb{E}[x_t x_{t+1}] = \rho\sigma^2$ almost surely and x_n^2 is integrable, $\alpha^* \rightarrow 1/\sigma^2$ and $\min_{\alpha} \mathcal{L}(\alpha) \rightarrow 0$. \square

Remark H.2 (Warm start vs. global optimum). *The optimization above is restricted to the asymptotic ray $b = [0, 1]^\top$, $A = [\alpha, 0]^\top$. It serves as a computational warm-up to practice Isserlis-based moment calculations and to quantify the finite-sample gap. The global optimum over all (b, A) may differ, but this warm start already converges to the linear-regression limit as $n \rightarrow \infty$.*

Auxiliary lemmas used in Appendix H.1

Theorem H.3 (Isserlis' Theorem (Wick's Formula) [Iss18]). *Let (X_1, \dots, X_n) be a zero-mean multivariate normal random vector.*

- If n is odd, i.e., $n = 2m + 1$, then

$$\mathbb{E}[X_1 X_2 \cdots X_{2m+1}] = 0.$$

- If n is even, i.e., $n = 2m$, then

$$\mathbb{E}[X_1 X_2 \cdots X_{2m}] = \sum_{p \in \mathcal{P}_n} \prod_{\{i, j\} \in p} \mathbb{E}[X_i X_j],$$

where \mathcal{P}_n denotes the set of all possible pairwise partitions (perfect matchings) of $\{1, 2, \dots, 2m\}$.

H.2 A finite-sample optimality gap for one-layer LSA

Goal. We prove that for any fixed sample size n , the best one-layer LSA readout on Hankel inputs *cannot* match linear regression on the last p lags. The argument rewrites the readout as a quadratic form in a Kronecker-lifted feature, solves the induced convex problem in closed form, and identifies a strictly positive Schur-complement gap. In other words, this section provides the first rigorous separation between LSA and linear regression: the gap is not an artifact of optimization, but a structural property of the linear self attention.

Setup (recalled). Let $\{x_t\}$ be a zero-mean stationary $\text{AR}(p)$ process as in Definition B.2. For $n \geq p$, let H_n be the Hankel matrix from Definition B.5 and put

$$G := \frac{1}{n} H_n M H_n^\top = \frac{1}{n} \sum_{i=1}^{n-p} x^{(i)} x^{(i)\top} \in \mathbb{R}^{(p+1) \times (p+1)}, \quad M := \text{diag}(I_{n-p}, 0).$$

Denote the prediction window $x := x_{n-p+1:n} \in \mathbb{R}^p$ and $y := x_{n+1} = \rho^\top x + \varepsilon_{n+1}$ with $\mathbb{E}[\varepsilon_{n+1}] = 0$, $\mathbb{E}[\varepsilon_{n+1}^2] = \sigma_\varepsilon^2$ and $\varepsilon_{n+1} \perp (G, x)$. Given parameters $b \in \mathbb{R}^{p+1}$ and $A \in \mathbb{R}^{(p+1) \times p}$, the one-layer LSA readout at the prediction slot is

$$\hat{x}_{n+1}(b, A) = b^\top G A x. \quad (4)$$

Kronecker reparameterization. Let D_{p+1} be the $(p+1)$ -dimensional duplication matrix so that $\text{vec}(G) = D_{p+1} \text{vech}(G)$. Using $\text{vec}(AXB) = (B^\top \otimes A) \text{vec}(X)$ and the mixed-product rule,

$$x^\top (A^\top G b) = ((\text{vech } G)^\top D_{p+1}^\top \otimes x^\top) (b \otimes \text{vec}(A^\top)) = ((\text{vech } G)^\top \otimes x^\top) \tilde{\eta},$$

where

$$\tilde{\eta} := (D_{p+1}^\top \otimes I_p) (b \otimes \text{vec}(A^\top)) \in \mathbb{R}^{qp}, \quad q := \frac{(p+1)(p+2)}{2}.$$

Introduce the lifted feature and its moments

$$Z := (\text{vech } G) \otimes x \in \mathbb{R}^{qp}, \quad \tilde{S} := \mathbb{E}[ZZ^\top], \quad \tilde{r} := \mathbb{E}[Zx^\top], \quad \Gamma_p := \mathbb{E}[xx^\top].$$

Then the mean-squared error decomposes as a strictly convex quadratic in $\tilde{\eta}$:

$$\begin{aligned} \mathcal{L}(b, A) &:= \mathbb{E}[(\hat{x}_{n+1}(b, A) - y)^2] \\ &= \sigma_\varepsilon^2 + \rho^\top \Gamma_p \rho + \tilde{\eta}^\top \tilde{S} \tilde{\eta} - 2 \tilde{\eta}^\top \tilde{r} \rho. \end{aligned} \quad (5)$$

Two technical facts we will establish and use.

(F1) The block second-moment matrix

$$\Sigma^\otimes := \mathbb{E} \left[\begin{pmatrix} Z \\ x \end{pmatrix} \begin{pmatrix} Z \\ x \end{pmatrix}^\top \right] = \begin{pmatrix} \tilde{S} & \tilde{r} \\ \tilde{r}^\top & \Gamma_p \end{pmatrix} \text{ is strictly positive definite.}$$

Equivalently, $\tilde{S} \succ 0$ and the Schur complement $\Gamma_p - \tilde{r}^\top \tilde{S}^{-1} \tilde{r} \succ 0$.

(F2) The unconstrained minimizer of (5) is $\tilde{\eta}^* = \tilde{S}^{-1} \tilde{r} \rho$ with minimum value

$$\mathcal{L}_{\min} = \sigma_\varepsilon^2 + \rho^\top \Gamma_p \rho - \rho^\top \tilde{r}^\top \tilde{S}^{-1} \tilde{r} \rho.$$

Because the original parameters (b, A) satisfy the rank-one Kronecker constraint $\tilde{\eta} = (D_{p+1}^\top \otimes I_p)(b \otimes \text{vec}(A^\top))$, their achievable risk is *no smaller* than \mathcal{L}_{\min} .

The core of the proof is thus (F1); (F2) is elementary convex optimization once (F1) holds.

Step 1: strict positive definiteness of a basic block

We begin by showing that the basic statistics at time n already enjoy strict nondegeneracy.

Lemma H.4 (Strict covariance of $(\text{vech } G, x)$). *Let $g := \text{vech } G \in \mathbb{R}^q$ and $x := x_{n-p+1:n} \in \mathbb{R}^p$. Then the covariance matrix*

$$\text{Cov}([g^\top, x^\top]^\top) \succ 0.$$

Proof. Write $Z_0 := [g^\top, x^\top]^\top$ and suppose, for contradiction, that there exists a nonzero vector v with $\text{Var}(v^\top Z_0) = 0$. We will force all coordinates of v to be zero by an *innovation-by-innovation* elimination. Let $\mathcal{F}_t := \sigma(\varepsilon_s : s \leq t)$. Proceed by traversing the rearranged vector Z_0 as shown below, in a *row-wise from bottom to top*, eliminating coefficients accordingly.

$$\tilde{Z}_0 = \left[\begin{array}{cccccc} \sum_{m=1}^{n-p} x_m^2 & & & & & \\ \sum_{m=1}^{n-p} x_m x_{m+1} & \sum_{m=1}^{n-p} x_{m+1}^2 & & & & \\ \sum_{m=1}^{n-p} x_m x_{m+2} & \sum_{m=1}^{n-p} x_{m+1} x_{m+2} & \sum_{m=1}^{n-p} x_{m+2}^2 & & & \\ \vdots & \vdots & \vdots & \ddots & & \\ \sum_{m=1}^{n-p} x_m x_{m+p} & \sum_{m=1}^{n-p} x_{m+1} x_{m+p} & \sum_{m=1}^{n-p} x_{m+2} x_{m+p} & \cdots & \sum_{m=1}^{n-p} x_{m+p}^2 & \end{array} \right] \begin{array}{l} x_{n-p+1} \\ x_{n-p+2} \\ \vdots \\ x_n \end{array}$$

Bottom block (involving x_n). The last row of the Hankel Gram contributes, among others, the terms $\sum_{m=1}^{n-p} x_{m+p}^2$ and $\sum_{m=1}^{n-p} x_{m+p-1}x_{m+p}$, whose final summands are x_n^2 and $x_{n-1}x_n$. Collecting the coefficients in v that multiply $\{x_n^2, x_{n-1}x_n, \dots, x_{n-p}x_n, x_n\}$, we can write

$$v^\top Z_0 = (\text{terms } \mathcal{F}_{n-1}\text{-measurable}) + (u^\top x_{n-p:n-1} + a x_n + c) x_n,$$

for some reals a, c and a vector $u \in \mathbb{R}^p$ determined by v . Since $x_n = \rho^\top x_{n-p:n-1} + \varepsilon_n$ with $\varepsilon_n \perp \mathcal{F}_{n-1}$ and ε_n independent of all earlier innovations, the conditional variance is

$$\text{Var}(v^\top Z_0 \mid \mathcal{F}_{n-1}) = \text{Var}((u^\top x_{n-p:n-1} + c)\varepsilon_n + a\varepsilon_n^2 \mid \mathcal{F}_{n-1}).$$

If $a \neq 0$ on a set of positive probability and ε_n has finite fourth moment (true e.g. for Gaussian innovations), then this conditional variance is > 0 on that set; hence $\text{Var}(v^\top Z_0) > 0$, a contradiction. Thus $a = 0$ a.s. With $a = 0$, the conditional variance reduces to $\text{Var}((u^\top x_{n-p:n-1} + c)\varepsilon_n \mid \mathcal{F}_{n-1}) = (u^\top x_{n-p:n-1} + c)^2 \sigma_\varepsilon^2$, forcing $u^\top x_{n-p:n-1} + c = 0$ a.s. By Lemma H.10, this implies $u = 0$ and $c = 0$. Hence *all* coefficients of v that touch x_n vanish.

Induction upward. Assume we have eliminated all coefficients attached to $x_n, x_{n-1}, \dots, x_{n-r+1}$ and to every Gram entry that involves these variables (this means we have removed the last r block-rows of the lower-triangular tableau of the sums defining g). Focus on the remaining first time that appears, x_{n-r} . Exactly the same conditioning on \mathcal{F}_{n-r-1} , writing $x_{n-r} = \phi^\top x_{n-r-p:n-r-1} + \varepsilon_{n-r}$, shows that the coefficient of x_{n-r}^2 must be 0, and then the linear coefficient of x_{n-r} must be 0. By Lemma H.10 again, *all* coefficients in v that touch x_{n-r} vanish.

Proceeding for $r = 1, \dots, p$ removes all entries of v associated with x and with the last p block-rows of g . Finally, the block that involves no recent x 's also collapses by the same argument (conditioning on \mathcal{F}_t at the appropriate times). We conclude $v = 0$, contradicting the assumption. Therefore $\text{Cov}(Z_0) \succ 0$. \square

Lemma H.5 (Two linear-algebra tools). (i) If $\Sigma = \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix} \in \mathbb{R}^{(m+n) \times (m+n)}$ is positive definite, then the Schur complement $\Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA} \succ 0$. (ii) If X is square-integrable with $\text{Cov}(X) \succ 0$ then, for every nonzero v , $\text{Var}(v^\top X) > 0$.

Proof. (i) is standard; see, e.g., any matrix analysis text. (ii) is immediate from $v^\top \text{Cov}(X)v = \text{Var}(v^\top X)$. \square

Step 2: lifting to the Kronecker level

We now show that the lift $Z = (\text{vech } G) \otimes x$ is also strictly nondegenerate in the block sense.

Lemma H.6 (Strict PD of the Kronecker-lifted block). With $g := \text{vech } G$, $x := x_{n-p+1:n}$ and $Z := g \otimes x$,

$$\Sigma^\otimes = \begin{pmatrix} \tilde{S} & \tilde{r} \\ \tilde{r}^\top & \Gamma_p \end{pmatrix} = \mathbb{E} \left[\begin{pmatrix} Z \\ x \end{pmatrix} \begin{pmatrix} Z \\ x \end{pmatrix}^\top \right] \succ 0.$$

Proof. Take any $(u, w) \neq (0, 0)$ with $u \in \mathbb{R}^{qp}$, $w \in \mathbb{R}^p$, and reshape u into a matrix $U \in \mathbb{R}^{q \times p}$ so that $u = \text{vec}(U)$. Consider the scalar

$$Y := u^\top Z + w^\top x = \sum_{s=1}^p x_s \left(w_s + \sum_{\ell=1}^q U_{\ell s} g_\ell \right) = x^\top (w + Ug).$$

Condition on x . Using the tower property,

$$\text{Var}(Y) = \mathbb{E}[\text{Var}(Y \mid x)] + \text{Var}(\mathbb{E}[Y \mid x]) \geq \mathbb{E}[\text{Var}(x^\top (Ug) \mid x)].$$

Given x , x is a deterministic vector and g is still random. Hence

$$\text{Var}(x^\top (Ug) \mid x) = x^\top U \text{Cov}(g \mid x) U^\top x.$$

By Lemma H.4 and the Schur-complement Lemma H.5(i),

$$\text{Cov}(g \mid x) = \text{Cov}(g) - \text{Cov}(g, x) \Gamma_p^{-1} \text{Cov}(x, g) \succ 0.$$

Therefore, for any $U \neq 0$, $x^\top U \text{Cov}(g \mid x) U^\top x > 0$ on a set of positive probability (because $\Gamma_p \succ 0$ and x is non-degenerate); taking expectations yields $\text{Var}(Y) > 0$. If instead $U = 0$ then $u = 0$ and $Y = w^\top x$; since $\Gamma_p \succ 0$, Lemma H.5(ii) implies $\text{Var}(Y) > 0$ unless $w = 0$. Thus no nonzero (u, w) can make $\text{Var}(Y) = 0$, which proves $\Sigma^\otimes \succ 0$. \square

Step 3: the gap via a Schur complement

We are ready to state and prove the main result.

Theorem H.7 (Finite-sample optimality gap of one-layer LSA). *Let the setup above hold. Define*

$$\Delta := \Gamma_p - \tilde{r}^\top \tilde{S}^{-1} \tilde{r}.$$

Then

$$\min_{b,A} \mathbb{E}[(\hat{x}_{n+1}(b, A) - x_{n+1})^2] \geq \sigma_\varepsilon^2 + \rho^\top \Delta \rho, \quad \Delta \succ 0.$$

Equivalently,

$$\min_{b,A} \mathbb{E}[(\hat{x}_{n+1}(b, A) - x_{n+1})^2] \geq \min_w \mathbb{E}[(w^\top x - x_{n+1})^2] + \rho^\top \Delta \rho,$$

so one-layer LSA has a strictly positive excess risk over linear regression for any finite n .

Proof. By Lemma H.6, $\tilde{S} \succ 0$ and its Schur complement in Σ^\otimes is $\Gamma_p - \tilde{r}^\top \tilde{S}^{-1} \tilde{r} \succ 0$. Minimizing (5) over $\tilde{\eta}$ gives $\tilde{\eta}^* = \tilde{S}^{-1} \tilde{r} \rho$ and

$$\min_{\tilde{\eta}} \mathcal{L} = \sigma_\varepsilon^2 + \rho^\top \Gamma_p \rho - \rho^\top \tilde{r}^\top \tilde{S}^{-1} \tilde{r} \rho = \sigma_\varepsilon^2 + \rho^\top \Delta \rho.$$

Because (b, A) can realize only the rank-one Kronecker set of $\tilde{\eta}$, $\min_{b,A} \mathcal{L} \geq \min_{\tilde{\eta}} \mathcal{L}$, proving the bound. Strict positivity of the excess term follows from $\Delta \succ 0$. \square

Remark H.8 (Population limit and order of limits). *If G is replaced by the population covariance Γ_{p+1} , then $g = \text{vech}(\Gamma_{p+1})$ is deterministic. Writing $u := g$,*

$$\tilde{S} = (uu^\top) \otimes \Gamma_p, \quad \tilde{r} = u \otimes \Gamma_p \implies \tilde{r}^\top \tilde{S}^{-1} \tilde{r} = \Gamma_p,$$

so $\Delta = 0$ and the gap vanishes. For finite n , \tilde{S} is strictly PD and $\Delta \succ 0$; taking $n \rightarrow \infty$ before inverting collapses the gap, illustrating an order-of-limits effect. As shown in Proposition G.14, in the asymptotic regime we can indeed prove that the one-layer LSA readout exactly recovers the Bayes-optimal linear predictor in the limit.

Theorem H.9 (Uniform excess-risk over a parameter family). *Fix $0 < r < R$ and $\mathcal{R} := \{\rho \in \mathbb{R}^p : r < \|\rho\|_2 < R\}$. Set $\lambda_{\min} := \inf_{\rho \in \mathcal{R}} \lambda_{\min}(\Delta(\rho))$. Then, uniformly for all $\rho \in \mathcal{R}$,*

$$\min_{b,A} \mathbb{E}[(\hat{x}_{n+1}(b, A) - x_{n+1})^2] \geq \sigma_\varepsilon^2 + \lambda_{\min} r^2.$$

Proof. By Theorem H.7, the excess is $\rho^\top \Delta(\rho) \rho$ with $\Delta(\rho) \succ 0$ for each ρ . Continuity of $\rho \mapsto \Delta(\rho)$ and compactness of $\overline{\mathcal{R}} = \{\rho : r \leq \|\rho\|_2 \leq R\}$, the Extreme Value Theorem (Theorem H.11) ensures that $\lambda_{\min}(\Delta(\rho))$ attains a strictly positive minimum on $\overline{\mathcal{R}}$. Hence $\rho^\top \Delta(\rho) \rho \geq \lambda_{\min} \|\rho\|_2^2 \geq \lambda_{\min} r^2$. \square

Auxiliary lemmas used in Appendix H.2

Lemma H.10 (No non-trivial zero-variance combination of consecutive samples). *For any integers i and $k \geq 1$ and any coefficients c_1, \dots, c_k ,*

$$Y := \sum_{j=1}^k c_j x_{i+j-1} = 0 \text{ a.s.} \implies c_1 = \dots = c_k = 0.$$

Proof. Let $\mathcal{F}_{i+k-2} := \sigma(\varepsilon_t : t \leq i+k-2)$. Write $x_{i+k-1} = \phi^\top x_{i+k-2:i-1} + \varepsilon_{i+k-1}$ with $\varepsilon_{i+k-1} \perp \mathcal{F}_{i+k-2}$. Conditioning,

$$\text{Var}(Y \mid \mathcal{F}_{i+k-2}) = c_k^2 \text{Var}(\varepsilon_{i+k-1}) = c_k^2 \sigma_\varepsilon^2.$$

If $Y = 0$ a.s., then $\text{Var}(Y \mid \mathcal{F}_{i+k-2}) = 0$ a.s., hence $c_k = 0$. Iterate backwards on k to conclude $c_1 = \dots = c_k = 0$. \square

Theorem H.11 (Extreme Value Theorem [Rud21]). *Let $K \subset \mathbb{R}^n$ be a nonempty compact set, and let $f : K \rightarrow \mathbb{R}$ be continuous. Then f is bounded on K , and there exist points $x_{\min}, x_{\max} \in K$ such that*

$$f(x_{\min}) = \inf_{x \in K} f(x), \quad f(x_{\max}) = \sup_{x \in K} f(x).$$

H.3 Order of the finite-sample gap

Goal. We quantify the finite-sample excess risk in Theorem H.7 and show it decays at rate $1/n$. The proof expands the lifted second moments to first order around their population (rank-one) limit and evaluates the Schur complement via a singular block inverse.

Setup (recalled). Let $\{x_t\}$ be a zero-mean stationary Gaussian AR(p) process as in Definition B.2, with absolutely summable autocovariances $\sum_{h \in \mathbb{Z}} |\gamma_h| < \infty$. For $n \geq p$, let $H_n = [x^{(1)} \dots x^{(n-p+1)}]$ be the Hankel matrix from Definition B.5, mask $M = \text{diag}(I_{n-p}, 0)$, and

$$G_n = \frac{1}{n} H_n M H_n^\top = \frac{1}{n} \sum_{m=1}^{n-p} x^{(m)} x^{(m)\top} \in \mathbb{R}^{(p+1) \times (p+1)}.$$

Let $x := x_{n-p+1:n} \in \mathbb{R}^p$, $\Gamma_{p+1} := \mathbb{E}[x^{(m)} x^{(m)\top}]$, $\Gamma_p := \mathbb{E}[x x^\top]$, and $u := \text{vech}(\Gamma_{p+1}) \in \mathbb{R}^q$ with $q = \frac{(p+1)(p+2)}{2}$. Define the lifted moments

$$S_n := \mathbb{E}[(\text{vec } G_n \otimes x)(\text{vec } G_n \otimes x)^\top], \quad r_n := \mathbb{E}[(\text{vec } G_n \otimes x) x^\top],$$

and their half-vectorized versions

$$\tilde{S}_n := \mathbb{E}[(\text{vech } G_n \otimes x)(\text{vech } G_n \otimes x)^\top], \quad \tilde{r}_n := \mathbb{E}[(\text{vech } G_n \otimes x) x^\top].$$

Lemma H.12 (First-order expansions of \tilde{S}_n and \tilde{r}_n). *Let L_{p+1} be the elimination matrix with $\text{vech}(A) = L_{p+1} \text{vec}(A)$ for symmetric A . Then, as $n \rightarrow \infty$ with p fixed,*

$$S_n = (\text{vec } \Gamma_{p+1})(\text{vec } \Gamma_{p+1})^\top \otimes \Gamma_p + \frac{1}{n} C_S^{(\text{vec})} + o(1/n), \quad (6)$$

$$r_n = (\text{vec } \Gamma_{p+1}) \otimes \Gamma_p + \frac{1}{n} C_r^{(\text{vec})} + o(1/n), \quad (7)$$

for deterministic $C_S^{(\text{vec})}, C_r^{(\text{vec})}$ depending only on $\{\gamma_h\}, p$. Consequently

$$\tilde{S}_n = (u u^\top) \otimes \Gamma_p + \frac{1}{n} C_S + o(1/n), \quad \tilde{r}_n = u \otimes \Gamma_p + \frac{1}{n} C_r + o(1/n),$$

with $C_S = (L_{p+1} \otimes I_p) C_S^{(\text{vec})} (L_{p+1} \otimes I_p)^\top$ and $C_r = (L_{p+1} \otimes I_p) C_r^{(\text{vec})}$. Moreover, for any orthonormal $Q = [u/\|u\|, Q_\perp]$ and $P := Q \otimes I_p$, writing $c := \|u\|^2$,

$$\begin{aligned} \hat{S}_n &:= P^\top \tilde{S}_n P = \begin{bmatrix} c \Gamma_p & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{n} \begin{bmatrix} C_{11} & B^\top \\ B & C \end{bmatrix} + o(1/n), \\ \hat{r}_n &:= P^\top \tilde{r}_n = \begin{bmatrix} \|u\| \Gamma_p \\ 0 \end{bmatrix} + \frac{1}{n} \begin{bmatrix} \delta \\ d \end{bmatrix} + o(1/n), \end{aligned} \quad (8)$$

where $\begin{bmatrix} C_{11} & B^\top \\ B & C \end{bmatrix} = P^\top C_S P$ and $\begin{bmatrix} \delta \\ d \end{bmatrix} = P^\top C_r$.

Proof. Stationarity gives $(\Gamma_{p+1})_{ij} = \gamma_{j-i}$ and $(\Gamma_p)_{st} = \gamma_{t-s}$ for indices $i, j, k, \ell \in \{1, \dots, p+1\}$ and $s, t \in \{1, \dots, p\}$. All variables are jointly Gaussian with zero mean; Isserlis' theorem is used throughout.

Computation of r_n . By linearity and $G_n = \frac{1}{n} \sum_{m=1}^{n-p} x^{(m)} x^{(m)\top}$,

$$r_n = \sum_{i,j,s,t} \mathbb{E}[G_{ij} x_s x_t] (e_j \otimes e_i \otimes e_s) e_t^\top, \quad \mathbb{E}[G_{ij} x_s x_t] = \frac{1}{n} \sum_{m=1}^{n-p} \mathbb{E}[x_i^{(m)} x_j^{(m)} x_s x_t],$$

with $x_i^{(m)} = x_{m+i-1}$. Let $a = x_{m+i-1}$, $b = x_{m+j-1}$, $c = x_{n-p+s}$, $d = x_{n-p+t}$. Isserlis yields

$$\begin{aligned} \mathbb{E}[abcd] &= \mathbb{E}[ab]\mathbb{E}[cd] + \mathbb{E}[ac]\mathbb{E}[bd] + \mathbb{E}[ad]\mathbb{E}[bc] \\ &= \gamma_{j-i}(\Gamma_p)_{st} + \gamma_{(n-p+s)-(m+i-1)} \gamma_{(n-p+t)-(m+j-1)} \\ &\quad + \gamma_{(n-p+t)-(m+i-1)} \gamma_{(n-p+s)-(m+j-1)}. \end{aligned}$$

With $k := n - p - m + 1 \in \{1, \dots, n - p\}$,

$$\mathbb{E}[x_i^{(m)} x_j^{(m)} x_s x_t] = \gamma_{j-i}(\Gamma_p)_{st} + \gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j}.$$

Summing over m ,

$$\mathbb{E}[G_{ij} x_s x_t] = \frac{n-p}{n} \gamma_{j-i}(\Gamma_p)_{st} + \frac{1}{n} \sum_{k=1}^{n-p} (\gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j}).$$

The first term equals $\gamma_{j-i}(\Gamma_p)_{st} + \frac{p}{n} \gamma_{j-i}(\Gamma_p)_{st}$. Since $\sum_h |\gamma_h| < \infty$, the partial sums $\sum_{k=1}^{n-p} \gamma_{k+a} \gamma_{k+b}$ are uniformly bounded for fixed a, b , and hence

$$\frac{1}{n} \sum_{k=1}^{n-p} (\gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j}) = \frac{1}{n} c_{ij,st}^{(r)} + o(1/n),$$

where

$$c_{ij,st}^{(r)} := \sum_{k=1}^{\infty} (\gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j})$$

converges absolutely. Note that

$$\begin{aligned} &\sum_{i,j,s,t} \gamma_{j-i}(\Gamma_p)_{st} (e_j \otimes e_i \otimes e_s) e_t^\top \\ &= \sum_{i,j,s,t} (\Gamma_{p+1})_{ij} (\Gamma_p)_{st} (e_j \otimes e_i) \otimes (e_s e_t^\top) \\ &= \sum_{i,j} (\Gamma_{p+1})_{ij} e_j \otimes e_i \otimes \left(\sum_{s,t} (\Gamma_p)_{st} e_s e_t^\top \right) \\ &= \text{vec}(\Gamma_{p+1}) \otimes \Gamma_p \end{aligned}$$

Therefore

$$r_n = (\text{vec} \Gamma_{p+1}) \otimes \Gamma_p + \frac{1}{n} \sum_{i,j,s,t} \left(-p \gamma_{j-i}(\Gamma_p)_{st} + c_{ij,st}^{(r)} \right) (e_j \otimes e_i \otimes e_s) e_t^\top + o(1/n),$$

which is (7) with $C_r^{(\text{vec})}$ defined by the bracketed coefficients.

Computation of S_n . By definition,

$$S_n = \sum_{i,j,k,\ell} \sum_{s,t} \mathbb{E}[G_{ij} G_{k\ell} x_s x_t] ((e_j \otimes e_i \otimes e_s) (e_\ell \otimes e_k \otimes e_t)^\top),$$

where

$$\mathbb{E}[G_{ij} G_{k\ell} x_s x_t] = \frac{1}{n^2} \sum_{m=1}^{n-p} \sum_{m'=1}^{n-p} \mathbb{E}[x_i^{(m)} x_j^{(m)} x_k^{(m')} x_\ell^{(m')} x_s x_t].$$

Let $a = x_{m+i-1}$, $b = x_{m+j-1}$, $c = x_{m'+k-1}$, $d = x_{m'+\ell-1}$, $e = x_{n-p+s}$, $f = x_{n-p+t}$. Isserlis for six variables decomposes into the term $\mathbb{E}[ef]\mathbb{E}[abcd]$ and the 12 cross pairings where e and/or f pair with $\{a, b, c, d\}$. For the four-variable factor,

$$\begin{aligned}\mathbb{E}[abcd] &= \gamma_{j-i} \gamma_{\ell-k} + \gamma_{(m+i-1)-(m'+k-1)} \gamma_{(m+j-1)-(m'+\ell-1)} \\ &\quad + \gamma_{(m+i-1)-(m'+\ell-1)} \gamma_{(m+j-1)-(m'+k-1)}.\end{aligned}$$

Let $h = m - m'$. Then

$$\mathbb{E}[abcd] = \gamma_{j-i} \gamma_{\ell-k} + \gamma_{i-k+h} \gamma_{j-\ell+h} + \gamma_{i-\ell+h} \gamma_{j-k+h}.$$

Averaging over m, m' ,

$$\begin{aligned}\frac{1}{n^2} \sum_{m, m'} \mathbb{E}[abcd] &= \gamma_{j-i} \gamma_{\ell-k} + \left(1 - \frac{(n-p)^2}{n^2}\right) \gamma_{j-i} \gamma_{\ell-k} \\ &\quad + \sum_{h=-(n-p-1)}^{n-p-1} \frac{n-p-|h|}{n^2} \left(\gamma_{i-k+h} \gamma_{j-\ell+h} + \gamma_{i-\ell+h} \gamma_{j-k+h} \right).\end{aligned}$$

Because $(n-p-|h|)/n^2 = (1/n) \cdot (1-|h|/(n-p)) \cdot \frac{n-p}{n}$ and $\sum_h |\gamma_h| < \infty$,

$$\frac{1}{n^2} \sum_{m, m'} \mathbb{E}[abcd] = \gamma_{j-i} \gamma_{\ell-k} + \frac{1}{n} c_{ij, k\ell}^{(S,0)} + o(1/n), \quad c_{ij, k\ell}^{(S,0)} := \sum_{h \in \mathbb{Z}} \left(\gamma_{i-k+h} \gamma_{j-\ell+h} + \gamma_{i-\ell+h} \gamma_{j-k+h} \right).$$

Multiplication by $(\Gamma_p)_{st}$ gives the leading block $\gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st}$, which matches $(\text{vec } \Gamma_{p+1}) (\text{vec } \Gamma_{p+1})^\top \otimes \Gamma_p$ entrywise.

Each cross pairing contributes a product of three covariances with at most linear dependence on m, m' . For instance, the pairing $\{e, a\}, \{f, b\}, \{c, d\}$ yields

$$\gamma_{(n-p+s)-(m+i-1)} \gamma_{(n-p+t)-(m+j-1)} \gamma_{(m'+k-1)-(m'+\ell-1)} = \gamma_{s-i+k} \gamma_{t-j+k} \gamma_{\ell-k},$$

after setting $k = n-p-m+1$. Summing over m, m' produces $\frac{1}{n} \left(\sum_{k=1}^{n-p} \gamma_{s-i+k} \gamma_{t-j+k} \right) \gamma_{\ell-k}$, which equals $\frac{1}{n}$ times a finite constant plus $o(1/n)$ by absolute summability through Toeplitz summation (see Lemma H.16). Enumerating all 12 cross pairings and collecting like terms gives the absolutely convergent series

$$\begin{aligned}c_{ij, k\ell; st}^{(S,1)} &= \sum_{q=1}^{\infty} \left[\gamma_{s-i+q} \gamma_{t-j+q} \gamma_{\ell-k} + \gamma_{s-i+q} \gamma_{t-k} \gamma_{j-\ell+q} + \gamma_{s-i+q} \gamma_{t-\ell} \gamma_{j-k+q} \right. \\ &\quad \left. + \gamma_{s-j+q} \gamma_{t-i+q} \gamma_{\ell-k} + \gamma_{s-j+q} \gamma_{t-k} \gamma_{i-\ell+q} + \gamma_{s-j+q} \gamma_{t-\ell} \gamma_{i-k+q} \right] \\ &\quad + \sum_{q=1}^{\infty} \left[\gamma_{t-i+q} \gamma_{s-j+q} \gamma_{\ell-k} + \gamma_{t-i+q} \gamma_{s-k} \gamma_{j-\ell+q} + \gamma_{t-i+q} \gamma_{s-\ell} \gamma_{j-k+q} \right. \\ &\quad \left. + \gamma_{t-j+q} \gamma_{s-i+q} \gamma_{\ell-k} + \gamma_{t-j+q} \gamma_{s-k} \gamma_{i-\ell+q} + \gamma_{t-j+q} \gamma_{s-\ell} \gamma_{i-k+q} \right].\end{aligned}$$

Boundary corrections of order $1/n$ proportional to $\gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st}$ are absorbed into the final constant. Consequently,

$$\mathbb{E}[G_{ij} G_{k\ell} x_s x_t] = \gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st} + \frac{1}{n} \left(c_{ij, k\ell}^{(S,0)} (\Gamma_p)_{st} + c_{ij, k\ell; st}^{(S,1)} \right) + o(1/n).$$

Substituting into the tensor expansion of S_n yields (6) with

$$C_S^{(\text{vec})} = \sum_{i, j, k, \ell} \sum_{s, t} \left(c_{ij, k\ell}^{(S,0)} (\Gamma_p)_{st} + c_{ij, k\ell; st}^{(S,1)} \right) ((e_j \otimes e_i \otimes e_s) (e_\ell \otimes e_k \otimes e_t)^\top).$$

Passing to vech. Since $\text{vech}(A) = L_{p+1} \text{vec}(A)$ for symmetric A , it follows that

$$\tilde{S}_n = (L_{p+1} \otimes I_p) S_n (L_{p+1} \otimes I_p)^\top, \quad \tilde{r}_n = (L_{p+1} \otimes I_p) r_n,$$

which, together with (6)–(7), gives the stated expansions with $S_\infty = (uu^\top) \otimes \Gamma_p$ and $r_\infty = u \otimes \Gamma_p$, and with the indicated C_S, C_r . Finally, for any orthonormal $Q = [u/\|u\|, Q_\perp]$ and $P = Q \otimes I_p$, the block forms for $\hat{S}_n = P^\top \tilde{S}_n P$ and $\hat{r}_n = P^\top \tilde{r}_n$ follow by inserting the expansions and collecting the top/orthogonal components; the leading block equals $\text{diag}(c \Gamma_p, 0)$ and the $1/n$ blocks are those of $P^\top C_S P$ and $P^\top C_r$. Dominated convergence (using $|\gamma_h| \leq C\beta^{|h|}$) justifies all $o(1/n)$ remainde \square

Lemma H.13 (Singular block inverse and first-order Schur complement). *In the basis of Lemma H.12, let*

$$\widehat{S}_n = \begin{bmatrix} A_0 & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{n} \begin{bmatrix} A_1 & B^\top \\ B & C \end{bmatrix} + o(1/n), \quad \widehat{r}_n = \begin{bmatrix} r_0 \\ 0 \end{bmatrix} + \frac{1}{n} \begin{bmatrix} \delta \\ d \end{bmatrix} + o(1/n),$$

with $A_0 = c\Gamma_p \succ 0$ and $r_0 = \|u\|\Gamma_p$. Then, for all large n ,

$$\widehat{r}_n^\top \widehat{S}_n^{-1} \widehat{r}_n = \Gamma_p + \frac{1}{n} \left[-\frac{1}{c} A_1 + \frac{1}{c} B^\top C^{-1} B - \frac{2}{\|u\|} B^\top C^{-1} d + d^\top C^{-1} d + \frac{2}{\|u\|} \text{Sym}(\delta) \right] + o(1/n),$$

where $\text{Sym}(M) = \frac{1}{2}(M + M^\top)$. Equivalently, in the original coordinates,

$$\begin{aligned} \widehat{r}_n^\top \widehat{S}_n^{-1} \widehat{r}_n &= \Gamma_p + \frac{1}{n} B_p + o(1/n), \\ B_p &:= -\frac{1}{c} A_1 + \frac{1}{c} B^\top C^{-1} B - \frac{2}{\|u\|} B^\top C^{-1} d + d^\top C^{-1} d + \frac{2}{\|u\|} \text{Sym}(\delta). \end{aligned} \quad (9)$$

Proof. Write the block decomposition of \widehat{S}_n from Lemma H.12 as

$$\widetilde{S}_n = \begin{bmatrix} A & E^\top \\ E & D \end{bmatrix}, \quad A = A_0 + \frac{1}{n} A_1 + o(1/n), \quad E = \frac{1}{n} B + o(1/n), \quad D = \frac{1}{n} C + o(1/n),$$

with $A_0 = c\Gamma_p \succ 0$. For large n , $D \succ 0$, and the block inverse formula gives

$$\widetilde{S}_n^{-1} = \begin{bmatrix} A^{-1} + A^{-1} E (D - E^\top A^{-1} E)^{-1} E^\top A^{-1} & -A^{-1} E (D - E^\top A^{-1} E)^{-1} \\ -(D - E^\top A^{-1} E)^{-1} E^\top A^{-1} & (D - E^\top A^{-1} E)^{-1} \end{bmatrix}.$$

Since $A^{-1} = A_0^{-1} - \frac{1}{n} A_0^{-1} A_1 A_0^{-1} + o(1/n)$ and $E^\top A^{-1} E = \frac{1}{n^2} B^\top A_0^{-1} B + o(1/n^2)$,

$$D - E^\top A^{-1} E = \frac{1}{n} C + o(1/n), \quad (D - E^\top A^{-1} E)^{-1} = n C^{-1} + o(n).$$

Substituting and collecting orders yields

$$\begin{aligned} (\widetilde{S}_n^{-1})_{11} &= A_0^{-1} - \frac{1}{n} A_0^{-1} A_1 A_0^{-1} + \frac{1}{n} A_0^{-1} B^\top C^{-1} B A_0^{-1} + o(1/n), \\ (\widetilde{S}_n^{-1})_{12} &= -A_0^{-1} B^\top C^{-1} + o(1), \\ (\widetilde{S}_n^{-1})_{22} &= n C^{-1} + o(n). \end{aligned}$$

Now expand $\widehat{r}_n = [r_0; 0] + \frac{1}{n} [\delta; d] + o(1/n)$ with $r_0 = \|u\|\Gamma_p$ and $A_0^{-1} = (1/c)\Gamma_p^{-1}$. Then

$$\widehat{r}_n^\top \widetilde{S}_n^{-1} \widehat{r}_n = r_0^\top (\widetilde{S}_n^{-1})_{11} r_0 + 2 r_0^\top (\widetilde{S}_n^{-1})_{12} \frac{1}{n} d + \frac{1}{n^2} d^\top (\widetilde{S}_n^{-1})_{22} d + \frac{2}{n} \text{Sym}(\delta^\top A_0^{-1} r_0) + o(1/n).$$

Each term is explicit:

$$\begin{aligned} r_0^\top A_0^{-1} r_0 &= \Gamma_p, \quad r_0^\top A_0^{-1} A_1 A_0^{-1} r_0 = \frac{1}{c} A_1, \quad r_0^\top A_0^{-1} B^\top C^{-1} B A_0^{-1} r_0 = \frac{1}{c} B^\top C^{-1} B, \\ 2 r_0^\top (\widetilde{S}_n^{-1})_{12} \frac{1}{n} d &= -\frac{2}{n} \cdot \frac{1}{\|u\|} B^\top C^{-1} d, \quad \frac{1}{n^2} d^\top (\widetilde{S}_n^{-1})_{22} d = \frac{1}{n} d^\top C^{-1} d + o(1/n), \\ \frac{2}{n} \text{Sym}(\delta^\top A_0^{-1} r_0) &= \frac{2}{n} \cdot \frac{1}{\|u\|} \text{Sym}(\delta). \end{aligned}$$

Combining yields

$$\widehat{r}_n^\top \widetilde{S}_n^{-1} \widehat{r}_n = \Gamma_p + \frac{1}{n} \left[-\frac{1}{c} A_1 + \frac{1}{c} B^\top C^{-1} B - \frac{2}{\|u\|} B^\top C^{-1} d + d^\top C^{-1} d + \frac{2}{\|u\|} \text{Sym}(\delta) \right] + o(1/n).$$

Since the orthogonal basis change preserves the Schur complement, the same expansion holds in the original coordinates, giving (9). \square

Theorem H.14 (First-order gap). *With $\Delta_n := \Gamma_p - \widehat{r}_n^\top \widetilde{S}_n^{-1} \widehat{r}_n$,*

$$\Delta_n = \frac{1}{n} B_p + o(1/n), \quad B_p := \frac{1}{c} A_1 - \frac{1}{c} B^\top C^{-1} B + \frac{2}{\|u\|} \text{Sym}(B^\top C^{-1} d - \delta) - d^\top C^{-1} d.$$

Hence the optimal one-layer LSA excess risk satisfies

$$\min_{b, A} \mathbb{E}[(\widehat{x}_{n+1}(b, A) - x_{n+1})^2] \geq \sigma_\varepsilon^2 + \rho^\top \Delta_n \rho = \sigma_\varepsilon^2 + \frac{1}{n} \rho^\top B_p \rho + o(1/n).$$

Moreover, $B_p \succeq 0$; if $B_p \succ 0$ (a generic nondegeneracy), then for any $r > 0$ there exist n_0 and $c_r > 0$ such that for all $n \geq n_0$ and all ρ with $\|\rho\| \geq r$,

$$\mathbb{E}[(\widehat{x}_{n+1}^{\text{LSA}} - x_{n+1})^2] \geq \mathbb{E}[(\widehat{x}_{n+1}^{\text{LR}} - x_{n+1})^2] + \frac{c_r}{n}.$$

Proof. By Lemma H.13, we have

$$\tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n = \Gamma_p + \frac{1}{n} \left[-\frac{1}{c} A_1 + \frac{1}{c} B^\top C^{-1} B - \frac{2}{\|u\|} B^\top C^{-1} d + d^\top C^{-1} d + \frac{2}{\|u\|} \text{Sym}(\delta) \right] + o(1/n).$$

Thus

$$\Delta_n := \Gamma_p - \tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n = \frac{1}{n} B_p + o(1/n),$$

with

$$B_p = \frac{1}{c} A_1 - \frac{1}{c} B^\top C^{-1} B + \frac{2}{\|u\|} \text{Sym}(B^\top C^{-1} d - \delta) - d^\top C^{-1} d.$$

By Lemma H.6, each $\Delta_n \succ 0$, hence $B_p = \lim_{n \rightarrow \infty} n \Delta_n \succeq 0$. The excess-risk bound follows from Theorem H.7:

$$\min_{b, A} \mathbb{E}[(\hat{x}_{n+1} - x_{n+1})^2] \geq \sigma_\varepsilon^2 + \rho^\top \Delta_n \rho = \sigma_\varepsilon^2 + \frac{1}{n} \rho^\top B_p \rho + o(1/n).$$

If $B_p \succ 0$, let $\lambda_0 = \lambda_{\min}(B_p) > 0$. For large n , $\|\Delta_n - (1/n)B_p\| \leq \lambda_0/(2n)$, hence $\rho^\top \Delta_n \rho \geq \frac{\lambda_0}{2n} \|\rho\|^2$. Therefore, for any $r > 0$, there exist n_0 and $c_r = \frac{1}{2} \lambda_0 r^2 > 0$ such that for all $n \geq n_0$ and all $\|\rho\| \geq r$,

$$\mathbb{E}[(\hat{x}_{n+1}^{\text{LSA}} - x_{n+1})^2] \geq \mathbb{E}[(\hat{x}_{n+1}^{\text{LR}} - x_{n+1})^2] + \frac{c_r}{n}.$$

□

Remark H.15 (Why the rate is $1/n$). *At the population limit $\tilde{S}_\infty = (uu^\top) \otimes \Gamma_p$ is rank-one along u . Finite n introduces $O(1/n)$ perturbations C_S, C_r that regularize the orthogonal directions, so the Schur complement $\Gamma_p - \tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n$ is $O(1/n)$. The overlap of Hankel windows is the source of these first-order terms.*

Auxiliary lemmas used in Appendix H.3

Lemma H.16 (Toeplitz-type summation). *Let $a : \mathbb{Z} \rightarrow \mathbb{R}$ (or \mathbb{C}) be absolutely summable, $\sum_{h \in \mathbb{Z}} |a_h| < \infty$. For $n \geq 1$ define*

$$S_n := \frac{1}{n^2} \sum_{m=1}^n \sum_{m'=1}^n a_{m-m'}.$$

Then

$$S_n = \frac{1}{n} \sum_{h \in \mathbb{Z}} \left(1 - \frac{|h|}{n}\right)_+ a_h = \frac{1}{n} \sum_{h \in \mathbb{Z}} a_h + \mathcal{O}\left(\frac{1}{n^2} \sum_{h \in \mathbb{Z}} |h| |a_h|\right) = \frac{1}{n} \sum_{h \in \mathbb{Z}} a_h + o(1/n).$$

Proof. Count the number of pairs $(m, m') \in \{1, \dots, n\}^2$ with difference $m - m' = h$; it equals $n - |h|$ if $|h| < n$ and 0 otherwise. Hence

$$\sum_{m, m'=1}^n a_{m-m'} = \sum_{h=-(n-1)}^{n-1} (n - |h|) a_h = n \sum_h \left(1 - \frac{|h|}{n}\right)_+ a_h.$$

Divide by n^2 and use absolute summability to obtain the stated bound.

H.4 A finite-sample gap for L stacked LSA layers (with monotone improvement)

Goal. For any fixed sample size n and depth $L \geq 1$, we show that the best L -layer linear self-attention (LSA) readout on Hankel inputs has a finite-sample excess risk over linear regression on the last p lags. To avoid unnecessary technicalities about duplicate features across layers, we work with the *convex relaxation* of the LSA parameters and allow singular second-moment matrices; the Moore–Penrose inverse then gives a clean *positive-semidefinite* (psd) gap. We also prove that the optimal risk is *monotone nonincreasing* in depth L .

Setup (layered). Let $\{x_t\}$ be a zero-mean stationary AR(p) process (Definition B.2). For $n \geq p$, let H_n be the Hankel matrix (Definition B.5), $M = \text{diag}(I_{n-p}, 0)$, and

$$G^{(0)} := \frac{1}{n} H_n M H_n^\top \in \mathbb{R}^{(p+1) \times (p+1)}.$$

Write $x := x_{n-p+1:n} \in \mathbb{R}^p$ and $y := x_{n+1} = \rho^\top x + \varepsilon_{n+1}$ with $\varepsilon_{n+1} \perp (G^{(0)}, x)$, $\mathbb{E}[\varepsilon_{n+1}] = 0$, $\mathbb{E}[\varepsilon_{n+1}^2] = \sigma_\varepsilon^2$. Initialize $y^{(0)} = 0$ and $H_n^{(0)} := H_n$. For $\ell = 0, \dots, L-1$ define the layer update

$$y^{(\ell+1)} = y^{(\ell)} + b^{(\ell)\top} G^{(\ell)} A^{(\ell)} x, \quad G^{(\ell+1)} = \frac{1}{n} H_n^{(\ell+1)} M (H_n^{(\ell+1)})^\top, \quad (10)$$

where $H_n^{(\ell+1)}$ coincides with H_n except that the last row uses the current layer's vector of entries whose last coordinate is $y^{(\ell+1)}$ (the mask M remains unchanged). The L -layer predictor is

$$\hat{x}_{n+1}^{(L)} = y^{(L)} = \sum_{\ell=0}^{L-1} b^{(\ell)\top} G^{(\ell)} A^{(\ell)} x. \quad (11)$$

A one-shot convex relaxation for depth L . Let $g^{(\ell)} := \text{vech } G^{(\ell)} \in \mathbb{R}^q$ with $q = \frac{(p+1)(p+2)}{2}$, and set the stacked Kronecker lift

$$Z^{[L]} := \begin{bmatrix} g^{(0)} \otimes x \\ \vdots \\ g^{(L-1)} \otimes x \end{bmatrix} \in \mathbb{R}^{d_L}, \quad d_L = Lqp.$$

For each layer, $b^{(\ell)\top} G^{(\ell)} A^{(\ell)} x$ can be written as $\eta^{(\ell)\top} (g^{(\ell)} \otimes x)$ with $\eta^{(\ell)} = (D_{p+1}^\top \otimes I_p) (b^{(\ell)} \otimes \text{vec}(A^{(\ell)\top}))$, and hence

$$\hat{x}_{n+1}^{(L)} = \eta^{[L]\top} Z^{[L]}, \quad \eta^{[L]} := [(\eta^{(0)})^\top, \dots, (\eta^{(L-1)})^\top]^\top.$$

Relaxing the rank-one Kronecker constraint on parameters leads to a linear regression of y on $Z^{[L]}$. Define the second moments

$$\tilde{S}_L := \mathbb{E}[Z^{[L]} Z^{[L]\top}], \quad \tilde{r}_L := \mathbb{E}[Z^{[L]} x^\top], \quad \Gamma_p := \mathbb{E}[xx^\top].$$

We allow \tilde{S}_L to be singular (duplicates across layers are harmless). The standard normal-equation calculation with the Moore-Penrose inverse gives

$$\min_{\eta^{[L]}} \mathbb{E}[(\eta^{[L]\top} Z^{[L]} - y)^2] = \sigma_\varepsilon^2 + \rho^\top \Gamma_p \rho - \rho^\top \tilde{r}_L^\top \tilde{S}_L^+ \tilde{r}_L \rho, \quad (12)$$

so the L -layer LSA family (which is a subset of the relaxed linear models) obeys the lower bound

$$\min_{\{b^{(\ell)}, A^{(\ell)}\}} \mathbb{E}[(\hat{x}_{n+1}^{(L)} - x_{n+1})^2] \geq \sigma_\varepsilon^2 + \rho^\top \Delta_{n,L} \rho, \quad \Delta_{n,L} := \Gamma_p - \tilde{r}_L^\top \tilde{S}_L^+ \tilde{r}_L \succeq 0. \quad (13)$$

Lemma H.17 (Why $\Delta_{n,L} \succeq 0$ even if \tilde{S}_L is singular). *Let $\Sigma_L := \mathbb{E}[[Z^{[L]}; x][Z^{[L]}; x]^\top] = \begin{bmatrix} \tilde{S}_L & \tilde{r}_L \\ \tilde{r}_L^\top & \Gamma_p \end{bmatrix}$. Then $\Sigma_L \succeq 0$, and the Moore-Penrose Schur complement $\Gamma_p - \tilde{r}_L^\top \tilde{S}_L^+ \tilde{r}_L$ is psd. Equivalently, $\Delta_{n,L} \succeq 0$ and equals the covariance of the best linear-prediction residual of x on $Z^{[L]}$.*

Proof. Σ_L is a covariance hence psd. For any matrix B , the prediction $Z^{[L]} \mapsto B^\top Z^{[L]}$ yields residual covariance $\Gamma_p - B^\top \tilde{r}_L - \tilde{r}_L^\top B + B^\top \tilde{S}_L B$. Minimizing over B (in the least-squares sense on the range of \tilde{S}_L) gives $B^* = \tilde{S}_L^+ \tilde{r}_L$ and residual covariance $\Gamma_p - \tilde{r}_L^\top \tilde{S}_L^+ \tilde{r}_L$, which is psd by definition of a covariance. \square

Depth helps: a simple embedding argument. We now show that the optimal risk is monotone in L ; the proof does not rely on invertibility nor on strictness.

Proposition H.18 (Monotone improvement with depth). *For every $L \geq 1$,*

$$\min_{\{b^{(\ell)}, A^{(\ell)}\}_{\ell=0}^L} \mathbb{E}[(\hat{x}_{n+1}^{(L+1)} - x_{n+1})^2] \leq \min_{\{b^{(\ell)}, A^{(\ell)}\}_{\ell=0}^{L-1}} \mathbb{E}[(\hat{x}_{n+1}^{(L)} - x_{n+1})^2],$$

where $\hat{x}_{n+1}^{(L)}$ is defined in (11) under the update rule (10). In particular, the best two-layer risk is no worse than the best one-layer risk:

$$\min_{b^{(0)}, A^{(0)}, b^{(1)}, A^{(1)}} \mathbb{E}[(\hat{x}_{n+1}^{(2)} - x_{n+1})^2] \leq \min_{b^{(0)}, A^{(0)}} \mathbb{E}[(\hat{x}_{n+1}^{(1)} - x_{n+1})^2].$$

Proof. Fix any parameter set $\{b^{(\ell)}, A^{(\ell)}\}_{\ell=0}^{L-1}$ for the L -layer model (11). Construct an $(L+1)$ -layer model by keeping the first L layers unchanged and appending a zero layer: $b^{(L)} = 0$, $A^{(L)} = 0$. Then $y^{(L+1)} = y^{(L)}$ and thus $\hat{x}_{n+1}^{(L+1)} = \hat{x}_{n+1}^{(L)}$, so the $(L+1)$ -layer loss equals the L -layer loss. Taking minima over the respective parameter sets yields the displayed inequality. The $L = 1 \rightarrow 2$ case is immediate, and the general case follows identically. \square

What we have (and what we do not claim). Equation (13) gives a finite-sample, depth- L gap

$$\mathbb{E}[(\hat{x}_{n+1}^{(L)} - x_{n+1})^2] \geq \mathbb{E}[(\hat{x}_{n+1}^{\text{LR}} - x_{n+1})^2] + \rho^\top \Delta_{n,L} \rho, \quad \Delta_{n,L} \succeq 0.$$

When duplicate features across layers make \tilde{S}_L singular, the bound remains valid via \tilde{S}_L^+ and interprets $\rho^\top \Delta_{n,L} \rho$ as the linear-projection residual variance. Under additional nondegeneracy, one can strengthen $\Delta_{n,L} \succ 0$ (strict gap) by proving that the stacked covariance Σ_L has a strictly positive Schur complement; this requires tracking how each layer injects new ε_n -directions into the last Hankel row and is omitted here for clarity.

Remarks. (i) The relaxation (12)–(13) can be written with a *deduplicated* stacked feature $\tilde{Z}^{[L]} = [g^{(0)} \otimes x, s^{(1)} \otimes x, \dots, s^{(L-1)} \otimes x]^\top$, where $s^{(\ell)}$ keeps only the new last-row/column monomials created at layer ℓ ; then $\tilde{S}_L := \mathbb{E}[\tilde{Z}^{[L]} \tilde{Z}^{[L]\top}]$ is typically invertible at finite n . All formulas remain the same with \tilde{S}_L^+ . (ii) In the population limit $n \rightarrow \infty$, $G^{(\ell)}$ concentrates around Γ_{p+1} , the stacked feature collapses to a rank-one Kronecker line, and $\Delta_{n,L} \rightarrow 0$; the order of limits matters, exactly as in the one-layer analysis.

I Chain-of-Thought (CoT) Rollout in TSF: Collapse-to-Mean and Error Compounding

We study the “free-running” (a.k.a. CoT) rollout where a predictor feeds its own outputs back as inputs instead of conditioning on future ground truth. For linear time-series models this produces a clean, analyzable dynamical system that (i) collapses to the mean and (ii) accumulates prediction error to the unconditional variance at an exponential rate. We also show that, for every forecast horizon, the Bayes (linear-regression) forecast is pointwise optimal, hence any linear self-attention (LSA) CoT rollout is uniformly worse and thus reaches a large-error regime *no later* than linear regression.

Setup. Let $\{x_t\}$ be a zero-mean, stable $\text{AR}(p)$ process as in Definition B.2, and let $A(\rho)$ denote the $p \times p$ companion matrix,

$$A(\rho) = \begin{pmatrix} \rho_1 & \rho_2 & \cdots & \rho_{p-1} & \rho_p \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix},$$

with spectral radius $\varrho(A(\rho)) < 1$. Write $s_t := (x_t, \dots, x_{t-p+1})^\top$. Then $s_{t+1} = A(\rho)s_t + \eta_{t+1}$ with $\eta_{t+1} := (\varepsilon_{t+1}, 0, \dots, 0)^\top$.

CoT rollout. Given an initial state $s_n = (x_n, \dots, x_{n-p+1})^\top$, a linear predictor with coefficients $w \in \mathbb{R}^p$ produces, in CoT mode, a noiseless recursion

$$\hat{s}_{t+1} = A(w)\hat{s}_t, \quad \hat{s}_0 = s_n,$$

with forecast $\hat{x}_{n+t} = e_1^\top \hat{s}_t$.

Proposition I.1 (Bayes multi-step forecast equals recursive rollout). *For any horizon $h \geq 1$, the Bayes forecast conditional on the history satisfies*

$$\hat{x}_{n+h}^* := \mathbb{E}[x_{n+h} \mid x_{1:n}] = \rho^\top \tilde{x}_{n+h-p:n+h-1},$$

where the rolled-out state \tilde{x}_k is defined recursively by

$$\tilde{x}_k = \begin{cases} x_k, & k \leq n, \\ \hat{x}_k^*, & k > n. \end{cases}$$

Equivalently, the optimal h -step forecast is obtained by repeatedly applying the one-step predictor with coefficients ρ and feeding predictions back in place of future observations.

Proof. Base case ($h = 1$). By the $\text{AR}(p)$ definition,

$$x_{n+1} = \rho^\top x_{n-p+1:n} + \varepsilon_{n+1}, \quad \varepsilon_{n+1} \perp x_{1:n}, \quad \mathbb{E}[\varepsilon_{n+1}] = 0,$$

so

$$\mathbb{E}[x_{n+1} \mid x_{1:n}] = \rho^\top x_{n-p+1:n} = \rho^\top \tilde{x}_{n-p+1:n}.$$

Induction step. Assume the claim holds up to horizon h . Then

$$x_{n+h+1} = \rho^\top x_{n+h-p+1:n+h} + \varepsilon_{n+h+1}.$$

Taking conditional expectation on $x_{1:n}$ yields

$$\mathbb{E}[x_{n+h+1} \mid x_{1:n}] = \rho^\top \mathbb{E}[x_{n+h-p+1:n+h} \mid x_{1:n}].$$

By the induction hypothesis, for indices $\leq n$ the conditional expectation equals the observed value, while for indices $> n$ it equals the Bayes forecasts \hat{x}^* , i.e. the recursively defined \tilde{x} . Therefore

$$\mathbb{E}[x_{n+h+1} \mid x_{1:n}] = \rho^\top \tilde{x}_{n+h-p+1:n+h}.$$

Conclusion. By induction, the identity holds for all horizons $h \geq 1$. Thus the Bayes multi-step forecast is exactly the recursive rollout of the one-step predictor with weight vector ρ . \square

Lemma I.2 (Exponential decay for any stable CoT). *If $\varrho(A(w)) < 1$, then for every consistent matrix norm there exist $C > 0$ and $\beta \in (0, 1)$ such that $\|\hat{s}_t\| \leq C\beta^t \|s_n\|$ and $\hat{x}_{n+t} \rightarrow 0$ exponentially fast.*

Proof. Unrolling the linear recursion gives $\hat{s}_t = A(w)^t s_n$. Because $\varrho(A(w)) < 1$, Lemma I.6 applies to $A(w)$: for any consistent operator norm there exist $C > 0$ and $\beta \in (0, 1)$ such that $\|A(w)^t\| \leq C\beta^t$ for all $t \in \mathbb{N}$. By submultiplicativity of the induced norm,

$$\|\hat{s}_t\| = \|A(w)^t s_n\| \leq \|A(w)^t\| \|s_n\| \leq C\beta^t \|s_n\|.$$

For the scalar forecast, $\hat{x}_{n+t} = e_1^\top \hat{s}_t$. Let $\|\cdot\|_*$ denote the dual norm of the chosen vector norm. Then $|\hat{x}_{n+t}| = |e_1^\top \hat{s}_t| \leq \|e_1\|_* \|\hat{s}_t\| \leq \|e_1\|_* C\beta^t \|s_n\|$. Since $\beta \in (0, 1)$, the right-hand side decays exponentially in t , establishing the claim. \square

Thus, *any* stable linear model (including the Bayes predictor and any LSA fit) collapses to the mean under CoT; the only question is how quickly its error compounds.

Bayes multi-step error (ground truth model). Let ψ_k be the impulse response of the $\text{AR}(p)$, i.e., $x_t = \sum_{k \geq 0} \psi_k \varepsilon_{t-k}$ with $\psi_0 = 1$ and $\sum_k \psi_k^2 < \infty$. The h -step Bayes forecast $\hat{x}_{n+h}^* = \mathbb{E}[x_{n+h} \mid x_{1:n}]$ equals the linear recursion with $w = \rho$ (no noise injected). The forecast error is classical:

$$\text{MSE}^*(h) := \mathbb{E}[(x_{n+h} - \hat{x}_{n+h}^*)^2] = \sigma_\varepsilon^2 \sum_{k=0}^{h-1} \psi_k^2. \quad (14)$$

Hence $\text{MSE}^*(h) \nearrow \sigma_\varepsilon^2 \sum_{k \geq 0} \psi_k^2 = \text{Var}(x_t)$ by Lemma I.7, and by Lemma I.8 the tail decays exponentially:

$$\text{Var}(x_t) - \text{MSE}^*(h) = \sigma_\varepsilon^2 \sum_{k \geq h} \psi_k^2 \leq \frac{C^2 \sigma_\varepsilon^2}{1 - \beta^2} \beta^{2h}, \quad \text{for some } C > 0, \beta \in (0, 1). \quad (15)$$

For $\text{AR}(1)$ this is exact: $\text{MSE}^*(h) = \sigma_\varepsilon^2 \sum_{k=0}^{h-1} \rho^{2k} = \sigma^2(1 - \rho^{2h})$, where $\sigma^2 = \sigma_\varepsilon^2/(1 - \rho^2)$.

Theorem I.3 (CoT collapse and compounding error). *For any stable $\text{AR}(p)$,*

$$\hat{x}_{n+t}^* \xrightarrow[t \rightarrow \infty]{} 0, \quad \mathbb{E}[(x_{n+t} - \hat{x}_{n+t}^*)^2] \nearrow \text{Var}(x_t),$$

with exponential tail (15). Thus CoT error accumulates to the process variance at an exponential rate determined by the spectrum of $A(\rho)$.

LSA (or any alternative) is uniformly dominated at every horizon. Fix a horizon h and let $\hat{x}_{n+h}^{\text{LSA}}$ be the CoT forecast delivered by any trained one-layer LSA model (or an L -layer stack run in CoT; the argument is identical). Since CoT is noiseless, $\hat{x}_{n+h}^{\text{LSA}}$ is a deterministic measurable function of the history $x_{1:n}$. By the L^2 projection property of the conditional expectation,

$$\mathbb{E}[(x_{n+h} - g(x_{1:n}))^2] = \text{MSE}^*(h) + \mathbb{E}[(\hat{x}_{n+h}^* - g(x_{1:n}))^2] \quad \forall g. \quad (16)$$

Plugging $g = \hat{x}_{n+h}^{\text{LSA}}$ yields the horizonwise dominance

$$\text{MSE}^{\text{LSA}}(h) := \mathbb{E}[(x_{n+h} - \hat{x}_{n+h}^{\text{LSA}})^2] \geq \text{MSE}^*(h), \quad (17)$$

with strict inequality unless $\hat{x}_{n+h}^{\text{LSA}}$ coincides with \hat{x}_{n+h}^* almost surely. Because one-layer LSA has a strict finite-sample gap (Section H.2), equality fails generically already at $h = 1$, and thus for all horizons.

Corollary I.4 (Earlier threshold crossing for LSA). *Fix any $\tau \in (0, 1)$ and define the failure horizon*

$$H_\tau(g) := \inf\{h \geq 1 : \mathbb{E}[(x_{n+h} - g_h(x_{1:n}))^2] \geq \tau \text{Var}(x_t)\}.$$

Then $H_\tau(\hat{x}^{\text{LSA}}) \leq H_\tau(\hat{x}^)$ for every τ , with strict inequality for all τ on a set of positive measure (whenever (17) is strict at some h). In words: for any error threshold, LSA under CoT reaches the large-error regime no later than the Bayes linear predictor.*

Quantitative rates. Combining Lemma I.2 with the orthogonality identity (16) shows that

$$\text{Var}(x_t) - \text{MSE}^{\text{LSA}}(h) \leq \text{Var}(x_t) - \text{MSE}^*(h) \leq \frac{C^2 \sigma_\varepsilon^2}{1 - \beta^2} \beta^{2h}, \quad \text{for some } C > 0, \beta \in (0, 1).$$

Hence whenever the left-hand side remains positive, it must also collapse to zero at least exponentially fast; if it turns negative (overshoot), Corollary I.4 guarantees that LSA in CoT still reaches the large-error regime strictly earlier and more severely than linear regression.

Remark I.5 (AR(1): closed forms and “rapid compounding”). For AR(1), $\text{MSE}^*(h) = \sigma^2(1 - \rho^{2h})$ so that the residual to the variance decays like ρ^{2h} . The “half-life” to reach 50% of the unconditional variance is $h_{1/2} = \log(1/2)/\log(\rho^2)$; e.g., with $\rho = 0.9$ one already has $\text{MSE}^*(5) \approx 0.65 \sigma^2$ and $\text{MSE}^*(10) \approx 0.88 \sigma^2$. This quantifies the rapid accumulation of CoT error even for the Bayes predictor; by (17), LSA CoT is uniformly worse at every horizon.

Takeaways. (i) Any linear CoT rollout collapses to the mean (Lemma I.2), so its long-horizon RMSE saturates at the unconditional standard deviation of the process. (ii) The Bayes/linear-regression forecast is *horizonwise* optimal (Theorem I.3 and (16)); any LSA CoT forecast is uniformly dominated at each horizon (17). (iii) Consequently, for any fixed error threshold, LSA reaches the large-error regime at least as early as linear regression (Corollary I.4). (iv) Both approaches exhibit exponential convergence of the error to the variance, with a rate governed by the spectral radius of the corresponding companion matrix; for AR(1) the entire trajectory is explicit.

Auxiliary lemmas used in Appendix I

Lemma I.6 (Exponential Decay from Spectral Radius Bound). Let $A \in \mathbb{R}^{p \times p}$ be a square matrix with spectral radius strictly less than one, i.e., $\varrho(A) < 1$. Then for any consistent matrix norm $\|\cdot\|$, there exist constants $C > 0$ and $\beta \in (0, 1)$ such that

$$\|A^t\| \leq C\beta^t \quad \text{for all } t \in \mathbb{N}.$$

Proof. By the Gelfand formula (see, e.g., [HJ94, Chapter 5]), we have

$$\varrho(A) = \lim_{t \rightarrow \infty} \|A^t\|^{1/t},$$

for any sub-multiplicative (i.e., consistent) matrix norm $\|\cdot\|$. Thus, for any $\epsilon > 0$ such that $\varrho(A) + \epsilon < 1$, there exists $t_0 \in \mathbb{N}$ such that

$$\|A^t\| \leq (\varrho(A) + \epsilon)^t =: \beta^t, \quad \forall t \geq t_0.$$

Define

$$C := \max\{1, \max_{0 \leq t < t_0} \frac{\|A^t\|}{\beta^t}\}.$$

Then for all $t \in \mathbb{N}$, we have $\|A^t\| \leq C\beta^t$ as claimed. \square

Lemma I.7 (Wold variance identity). For a stable AR(p) with Wold expansion $x_t = \sum_{k \geq 0} \psi_k \varepsilon_{t-k}$, where $\varepsilon_t \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2)$, the unconditional variance satisfies

$$\text{Var}(x_t) = \sigma_\varepsilon^2 \sum_{k \geq 0} \psi_k^2.$$

Proof. From the Wold representation $x_t = \sum_{k \geq 0} \psi_k \varepsilon_{t-k}$, we have $\mathbb{E}[x_t] = 0$ and

$$\text{Var}(x_t) = \mathbb{E}[x_t^2] = \mathbb{E} \left[\left(\sum_{k \geq 0} \psi_k \varepsilon_{t-k} \right)^2 \right].$$

Cross terms vanish because the ε_{t-k} are independent with mean zero, leaving $\sum_{k \geq 0} \psi_k^2 \mathbb{E}[\varepsilon_{t-k}^2] = \sigma_\varepsilon^2 \sum_{k \geq 0} \psi_k^2$. \square

Lemma I.8 (Exponential tail bound). *Let $A(\rho)$ be the AR(p) companion matrix with spectral radius $\varrho(A(\rho)) < 1$. Then the impulse response coefficients obey $|\psi_k| \leq C\beta^k$ for some $C > 0$ and $\beta \in (0, 1)$. Consequently,*

$$\sigma_\varepsilon^2 \sum_{k \geq h} \psi_k^2 \leq \frac{C^2 \sigma_\varepsilon^2}{1 - \beta^2} \beta^{2h}.$$

Proof. By state recursion, $\psi_k = e_1^\top A(\rho)^k e_1$. Because $\varrho(A(\rho)) < 1$, Lemma I.6 applies to $A(\rho)$: for any consistent operator norm there exist $C > 0$ and $\beta \in (0, 1)$ such that $\|A(\rho)^t\| \leq C\beta^t$ for all $t \in \mathbb{N}$. Hence $|\psi_k| \leq C\beta^k$. Thus,

$$\sum_{k \geq h} \psi_k^2 \leq \sum_{k \geq h} C^2 \beta^{2k} = \frac{C^2}{1 - \beta^2} \beta^{2h},$$

and multiplying by σ_ε^2 yields the claim. □

J De-Gaussifying the Gap: Linear Stationary Processes

Goal. We remove the Gaussian assumption and establish the same finite-sample excess-risk gap for one-layer LSA under a broad linear-stationary model. The strict gap requires only independence of innovations and finite moments; with absolutely summable autocovariances we also recover the $1/n$ first-order expansion.

Model. Let $\{x_t\}_{t \in \mathbb{Z}}$ be a zero-mean *linear stationary* process with Wold representation

$$x_t = \sum_{k \geq 0} \psi_k \varepsilon_{t-k}, \quad \sum_{k \geq 0} |\psi_k| < \infty, \quad (18)$$

where $\{\varepsilon_t\}$ are i.i.d. with $\mathbb{E}[\varepsilon_t] = 0$, $\mathbb{E}[\varepsilon_t^2] = \sigma_\varepsilon^2 > 0$, and with a symmetric distribution. We assume $\mathbb{E}[\varepsilon_t^4] < \infty$ and $\text{Var}(\varepsilon_t^2) < \infty$. Let $\gamma_h := \mathbb{E}[x_t x_{t+h}]$, so $\sum_{h \in \mathbb{Z}} |\gamma_h| < \infty$.

All Hankel/masking notation follows Section H.2:

$$G = \frac{1}{n} \sum_{m=1}^{n-p} x^{(m)} x^{(m)\top}, \quad x := x_{n-p+1:n} \in \mathbb{R}^p, \quad y := x_{n+1},$$

with the one-layer LSA predictor

$$\hat{x}_{n+1}^{\text{LSA}} = b^\top G A x, \quad b \in \mathbb{R}^{p+1}, \quad A \in \mathbb{R}^{(p+1) \times p}.$$

As in Section H.2, introduce

$$Z := (\text{vech } G) \otimes x, \quad \tilde{S} := \mathbb{E}[Z Z^\top], \quad \tilde{r} := \mathbb{E}[Z x^\top], \quad \Gamma_p := \mathbb{E}[x x^\top].$$

Linear regression predictor. For consistency with the Hankel construction, we restrict attention to the last p lags $x := x_{n-p+1:n} \in \mathbb{R}^p$ as regression covariates. The best linear predictor of $y := x_{n+1}$ from x is

$$y = w^* x + e_{n+1}, \quad \mathbb{E}[x e_{n+1}] = 0,$$

where $w^* \in \mathbb{R}^p$ is the least-squares coefficient vector and e_{n+1} is the linear prediction error. We denote the corresponding fitted value by

$$\hat{x}_{n+1}^{\text{LR}} := w^* x.$$

Lemma J.1 (Strict covariance of $(\text{vech } G, x)$ without Gaussianity). *Let $g := \text{vech } G$ and $x := x_{n-p+1:n}$. Under (18), $\text{Cov}([g^\top, x^\top]^\top) \succ 0$ for every finite n .*

Proof. Let $Z_0 = [g^\top, x^\top]^\top$. Suppose $\text{Var}(v^\top Z_0) = 0$ for some nonzero v . Traverse the tableau of Hankel-Gram sums from bottom (time n) upward. Collect coefficients of $\{x_n^2, x_{n-1}x_n, \dots, x_{n-p}x_n, x_n\}$ to write

$$v^\top Z_0 = U + V x_n + W x_n^2,$$

with U, V, W measurable w.r.t. $\mathcal{F}_{n-1} := \sigma(\varepsilon_s : s \leq n-1)$.

Write $x_n = \xi + \psi_0 \varepsilon_n$, where ξ is \mathcal{F}_{n-1} -measurable and $\varepsilon_n \perp \mathcal{F}_{n-1}$. By symmetry, $\text{Cov}(\varepsilon_n, \varepsilon_n^2) = 0$. Thus

$$\text{Var}(v^\top Z_0 \mid \mathcal{F}_{n-1}) = \text{Var}(V \psi_0 \varepsilon_n + W \psi_0^2 \varepsilon_n^2 \mid \mathcal{F}_{n-1}) = (V \psi_0)^2 \sigma_\varepsilon^2 + W^2 \psi_0^4 \text{Var}(\varepsilon_n^2).$$

Since both coefficients are strictly positive, this vanishes only if $V = W = 0$. Inductively repeating the elimination for x_{n-1}, x_{n-2}, \dots forces $v = 0$, a contradiction. Hence the covariance is strictly positive definite. \square

Lemma J.2 (Kronecker lift remains strictly PD). *With $Z = (\text{vech } G) \otimes x$ and $x = x_{n-p+1:n}$,*

$$\Sigma^\otimes := \mathbb{E} \begin{bmatrix} Z \\ x \end{bmatrix} \begin{bmatrix} Z \\ x \end{bmatrix}^\top = \begin{bmatrix} \tilde{S} & \tilde{r} \\ \tilde{r}^\top & \Gamma_p \end{bmatrix} \succ 0.$$

Proof. By Lemma J.1, $\text{Cov}([g, x]) \succ 0$; hence the conditional covariance $\text{Cov}(g | x) = \text{Cov}(g) - \text{Cov}(g, x)\Gamma_p^{-1}\text{Cov}(x, g) \succ 0$. For any nonzero $u = \text{vec}(U) \in \mathbb{R}^{qp}$ and $w \in \mathbb{R}^p$, put $Y := u^\top Z + w^\top x = x^\top(Ug + w)$. Then $\text{Var}(Y) \geq \mathbb{E}[x^\top U \text{Cov}(g | x) U^\top x] > 0$ unless $U = 0$; if $U = 0$ then $\text{Var}(Y) = \text{Var}(w^\top x) > 0$ since $\Gamma_p \succ 0$. Thus $\Sigma^\otimes \succ 0$. \square

Theorem J.3 (Strict finite-sample gap under linear stationarity). *Under the model above, for every finite n ,*

$$\min_{b, A} \mathbb{E} [(\hat{x}_{n+1}^{\text{LSA}} - \hat{x}_{n+1}^{\text{LR}})^2] = w^{*\top} \Delta_n w^*, \quad \Delta_n \succ 0.$$

Proof. As in (5), the LSA risk relative to the regression predictor can be written

$$\begin{aligned} \mathcal{L}(\eta) &= \mathbb{E} [(\hat{x}_{n+1}^{\text{LSA}} - \hat{x}_{n+1}^{\text{LR}})^2] \\ &= w^{*\top} \Gamma_p w^* + \eta^\top \tilde{S} \eta - 2\eta^\top \tilde{r} w^*. \end{aligned}$$

The minimizer is $\eta^* = \tilde{S}^{-1} \tilde{r} w^*$, giving the optimal value

$$w^{*\top} (\Gamma_p - \tilde{r}^\top \tilde{S}^{-1} \tilde{r}) w^* = w^{*\top} \Delta_n w^*.$$

By Lemma J.2, $\tilde{S} \succ 0$, hence $\Delta_n \succ 0$ by the Schur complement. \square

Remarks. (i) The gap above is defined relative to the best linear regression predictor $\hat{x}_{n+1}^{\text{LR}}$. (ii) If in addition the regression residual e_{n+1} is independent of (G, x) (as in an exact $\text{AR}(p)$ model with p lags), then the same gap translates directly to a strict excess risk gap relative to y .

Cumulant identities for linear processes. Let $\kappa_r := \text{cum}_r(\varepsilon_0)$ denote the order- r cumulant of ε_0 (finite for the orders we use). For any t_1, \dots, t_r ,

$$\text{cum}(x_{t_1}, \dots, x_{t_r}) = \kappa_r \sum_{u \in \mathbb{Z}} \psi_{t_1-u} \cdots \psi_{t_r-u}. \quad (19)$$

This follows from multilinearity of cumulants and independence of $\{\varepsilon_t\}$ (see, e.g., [Bri01, Theorem 2.3.2])

Lemma J.4 (Moment expansions via cumulants). *Assume $\sum_{h \in \mathbb{Z}} |\gamma_h| < \infty$, $\mathbb{E}|\varepsilon_t|^6 < \infty$ (so κ_4, κ_6 are finite). Let $u := \text{vech}(\Gamma_{p+1})$ and set $S_\infty := (uu^\top) \otimes \Gamma_p$, $r_\infty := u \otimes \Gamma_p$. For $n \rightarrow \infty$ with fixed p ,*

$$\tilde{S}_n = S_\infty + \frac{1}{n} C_S + o(1/n), \quad \tilde{r}_n = r_\infty + \frac{1}{n} C_r + o(1/n), \quad (20)$$

for finite matrices C_S, C_r determined by $\{\gamma_h\}$ and κ_4, κ_6 .

Proof. We work entrywise. Write indices $i, j, k, \ell \in \{1, \dots, p+1\}$, $s, t \in \{1, \dots, p\}$, and

$$a = x_{m+i-1}, \quad b = x_{m+j-1}, \quad c = x_{m'+k-1}, \quad d = x_{m'+\ell-1}, \quad e = x_{n-p+s}, \quad f = x_{n-p+t}.$$

Recall $G_{ij} = \frac{1}{n} \sum_{m=1}^{n-p} x_{m+i-1} x_{m+j-1}$. We analyze

$$(\tilde{r}_n)_{(ij,s),t} = \mathbb{E}[G_{ij} x_s x_t] = \frac{1}{n} \sum_{m=1}^{n-p} \mathbb{E}[a b e f], \quad (21)$$

$$(\tilde{S}_n)_{(ij,s),(k\ell,t)} = \mathbb{E}[G_{ij} G_{k\ell} x_s x_t] = \frac{1}{n^2} \sum_{m,m'=1}^{n-p} \mathbb{E}[a b c d e f]. \quad (22)$$

(I) *The r_n expansion.* By the moment-cumulant formula (see Lemma J.6), for four variables,

$$\mathbb{E}[a b e f] = \mathbb{E}[a b] \mathbb{E}[e f] + \mathbb{E}[a e] \mathbb{E}[b f] + \mathbb{E}[a f] \mathbb{E}[b e] + \text{cum}(a, b, e, f).$$

The pairwise terms equal

$$\gamma_{j-i}(\Gamma_p)_{st} + \gamma_{(n-p+s)-(m+i-1)} \gamma_{(n-p+t)-(m+j-1)} + \gamma_{(n-p+t)-(m+i-1)} \gamma_{(n-p+s)-(m+j-1)}.$$

Summing over m gives

$$\frac{n-p}{n} \gamma_{j-i}(\Gamma_p)_{st} + \frac{1}{n} \sum_{k=1}^{n-p} (\gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j}).$$

Because $\sum_h |\gamma_h| < \infty$, Toeplitz summation (see Lemma H.16) implies that the convolutions are uniformly bounded and converge; thus

$$\frac{n-p}{n} \gamma_{j-i}(\Gamma_p)_{st} = \gamma_{j-i}(\Gamma_p)_{st} - \frac{p}{n} \gamma_{j-i}(\Gamma_p)_{st},$$

and

$$\frac{1}{n} \sum_{k=1}^{n-p} (\gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j}) = \frac{1}{n} c_{ij,st}^{(r,2)} + o(1/n),$$

for some absolutely convergent constant

$$c_{ij,st}^{(r,2)} := \sum_{k=1}^{\infty} (\gamma_{k+s-i} \gamma_{k+t-j} + \gamma_{k+t-i} \gamma_{k+s-j}).$$

For the fourth-order cumulant, (19) with $r = 4$ yields

$$\text{cum}(a, b, e, f) = \kappa_4 \sum_{u \in \mathbb{Z}} \psi_{m+i-1-u} \psi_{m+j-1-u} \psi_{n-p+s-u} \psi_{n-p+t-u}.$$

Summing over m (equivalently $k = n - p - m + 1$) and using

$$\sum_{k \geq 1} \sum_u |\psi_{i-u+k} \psi_{j-u+k} \psi_{s-u} \psi_{t-u}| \leq \|\psi\|_{\ell_1}^4 < \infty$$

gives

$$\frac{1}{n} \sum_{m=1}^{n-p} \text{cum}(a, b, e, f) = \frac{1}{n} c_{ij,st}^{(r,4)} + o(1/n)$$

with an absolutely convergent constant $c_{ij,st}^{(r,4)} := \kappa_4 \sum_{k \geq 1} \sum_{u \in \mathbb{Z}} \psi_{i-u+k} \psi_{j-u+k} \psi_{s-u} \psi_{t-u}$. Collecting pieces and reorganizing in tensor form yields

$$r_n = (\text{vec } \Gamma_{p+1}) \otimes \Gamma_p + \frac{1}{n} C_r^{(\text{vec})} + o(1/n),$$

and therefore $\tilde{r}_n = (L_{p+1} \otimes I_p) r_n = r_\infty + \frac{1}{n} C_r + o(1/n)$.

(II) *The S_n expansion.* For

$$S_n = \sum_{i,j,k,\ell} \sum_{s,t} \mathbb{E}[G_{ij} G_{k\ell} x_s x_t] \left((e_j \otimes e_i \otimes e_s) (e_\ell \otimes e_k \otimes e_t)^\top \right).$$

Then

$$\mathbb{E}[G_{ij} G_{k\ell} x_s x_t] = \frac{1}{n^2} \sum_{m=1}^{n-p} \sum_{m'=1}^{n-p} \mathbb{E}[abcdef].$$

Sixth-order moment decomposition. By the moment-cumulant formula in Lemma J.6,

$$\mathbb{E}[abcdef] = \sum_{P \in \mathfrak{M}_3} \prod_{(u,v) \in P} \mathbb{E}[uv] + \sum_{\pi \in \Pi_{4,2}} \text{cum}_4(\pi^{(4)}) \mathbb{E}(\pi^{(2)}) + \text{cum}_6(a, b, c, d, e, f), \quad (23)$$

where \mathfrak{M}_3 is the set of the 15 perfect matchings of $\{a, b, c, d, e, f\}$, $\Pi_{4,2}$ is the set of the 15 partitions into a 4-block and a 2-block, $\pi^{(4)}$ denotes the 4-tuple in the 4-block and $\pi^{(2)}$ the paired variables. Write $\gamma_h := \mathbb{E}[x_t x_{t+h}]$.

(a) Triple-pairings. The three pairings that keep (e, f) together are

$$P_0 = \{(a, b), (c, d), (e, f)\}, \quad P_1 = \{(a, c), (b, d), (e, f)\}, \quad P_2 = \{(a, d), (b, c), (e, f)\}.$$

The leading pairing P_0 contributes

$$\frac{1}{n^2} \sum_{m, m'} \gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st} = \gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st} + \frac{1}{n} c_{ij, k\ell; st}^{(S, \text{bd})} + o(1/n),$$

with

$$c_{ij, k\ell; st}^{(S, \text{bd})} = -2p \gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st}. \quad (24)$$

The two additional pairings P_1, P_2 yield, after the change of variable $h = m - m'$ and Toeplitz summation (see Lemma H.16),

$$\frac{1}{n^2} \sum_{m, m'} \left(\gamma_{i-k+h} \gamma_{j-\ell+h} + \gamma_{i-\ell+h} \gamma_{j-k+h} \right) (\Gamma_p)_{st} = \frac{1}{n} c_{ij, k\ell; st}^{(S, 0)} + o(1/n),$$

where

$$c_{ij, k\ell; st}^{(S, 0)} := \sum_{h \in \mathbb{Z}} \left(\gamma_{i-k+h} \gamma_{j-\ell+h} + \gamma_{i-\ell+h} \gamma_{j-k+h} \right) (\Gamma_p)_{st} \quad (\text{absolutely convergent}). \quad (25)$$

Therefore, the total contribution of the three pairings with (e, f) paired is

$$\gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st} + \frac{1}{n} \left(c_{ij, k\ell; st}^{(S, \text{bd})} + c_{ij, k\ell; st}^{(S, 0)} \right) + o(1/n).$$

All other 12 pairings necessarily contain at least one cross-pair between $\{a, b, c, d\}$ and $\{e, f\}$. After the change of variable $q := n - p - m + 1$ (or $q := n - p - m' + 1$ as appropriate) and absolute summability of $\{\gamma_h\}$, each such term equals $\frac{1}{n}$ times a finite constant plus $o(1/n)$. Collecting the 12 distinct cross-pairings (those where e or f pairs with one of a, b, c, d) gives the *explicit* constant via Toeplitz summation (see Lemma H.16)

$$\begin{aligned} c_{ij, k\ell; st}^{(S, 2)} := \sum_{q=1}^{\infty} & \left[\gamma_{s-i+q} \gamma_{t-j+q} \gamma_{\ell-k} + \gamma_{s-i+q} \gamma_{t-k} \gamma_{j-\ell+q} + \gamma_{s-i+q} \gamma_{t-\ell} \gamma_{j-k+q} \right. \\ & + \gamma_{s-j+q} \gamma_{t-i+q} \gamma_{\ell-k} + \gamma_{s-j+q} \gamma_{t-k} \gamma_{i-\ell+q} + \gamma_{s-j+q} \gamma_{t-\ell} \gamma_{i-k+q} \\ & + \gamma_{t-i+q} \gamma_{s-j+q} \gamma_{\ell-k} + \gamma_{t-i+q} \gamma_{s-k} \gamma_{j-\ell+q} + \gamma_{t-i+q} \gamma_{s-\ell} \gamma_{j-k+q} \\ & \left. + \gamma_{t-j+q} \gamma_{s-i+q} \gamma_{\ell-k} + \gamma_{t-j+q} \gamma_{s-k} \gamma_{i-\ell+q} + \gamma_{t-j+q} \gamma_{s-\ell} \gamma_{i-k+q} \right]. \end{aligned}$$

Therefore the total contribution of triple-pairings is

$$\gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st} + \frac{1}{n} c_{ij, k\ell; st}^{(S, \text{bd})} + \frac{1}{n} c_{ij, k\ell; st}^{(S, 0)} + \frac{1}{n} c_{ij, k\ell; st}^{(S, 2)} + o(1/n). \quad (26)$$

(b) $\{4, 2\}$ partitions. For linear processes $x_t = \sum_{r \in \mathbb{Z}} \psi_{t-r} \varepsilon_r$ with i.i.d. innovations, the fourth cumulant satisfies $\text{cum}_4(x_{t_1}, x_{t_2}, x_{t_3}, x_{t_4}) = \kappa_4 \sum_{r \in \mathbb{Z}} \psi_{t_1-r} \psi_{t_2-r} \psi_{t_3-r} \psi_{t_4-r}$, where $\kappa_4 = \text{cum}_4(\varepsilon)$ and $\sum_k |\psi_k| < \infty$. Define the absolutely convergent series

$$S_{ab}(r) := \sum_{q \in \mathbb{Z}} \psi_{q+i-1-r} \psi_{q+j-1-r}, \quad S_{cd}(r) := \sum_{q \in \mathbb{Z}} \psi_{q+k-1-r} \psi_{q+\ell-1-r}.$$

By stationarity and Toeplitz summation, only the three families of partitions in which the 4-block contains either $\{a, b\}$ or $\{c, d\}$ contribute at order $1/n$; all other $\{4, 2\}$ partitions are $o(1/n)$. The non-vanishing $1/n$ constants are

$$\begin{aligned} c_{ij, k\ell; st}^{(S, 4)} := \kappa_4 \sum_{r \in \mathbb{Z}} & \left[\gamma_{t-s} S_{ab}(r) S_{cd}(r) + \gamma_{\ell-k} S_{ab}(r) \psi_{s-r} \psi_{t-r} \right. \\ & \left. + \gamma_{j-i} S_{cd}(r) \psi_{s-r} \psi_{t-r} \right]. \end{aligned} \quad (27)$$

(c) Sixth-order cumulant. Using $\text{cum}_6(x_{t_1}, \dots, x_{t_6}) = \kappa_6 \sum_{r \in \mathbb{Z}} \prod_{u=1}^6 \psi_{t_u-r}$ with $\kappa_6 = \text{cum}_6(\varepsilon)$, the double sum over (m, m') reduces (by Toeplitz summation) to

$$\frac{1}{n} c_{ij,kl;st}^{(S,6)} + o(1/n), \quad c_{ij,kl;st}^{(S,6)} := \kappa_6 \sum_{r \in \mathbb{Z}} S_{ab}(r) S_{cd}(r) \psi_{s-r} \psi_{t-r}. \quad (28)$$

(d) Collecting the pieces. Combining (26), (27) and (28) in (23) yields

$$\mathbb{E}[G_{ij} G_{kl} x_s x_t] = \gamma_{j-i} \gamma_{\ell-k} (\Gamma_p)_{st} + \frac{1}{n} \left(c_{ij,kl;st}^{(S,\text{bd})} + c_{ij,kl;st}^{(S,0)} + c_{ij,kl;st}^{(S,2)} + c_{ij,kl;st}^{(S,4)} + c_{ij,kl;st}^{(S,6)} \right) + o(1/n).$$

Therefore

$$S_n = (\text{vec } \Gamma_{p+1}) (\text{vec } \Gamma_{p+1})^\top \otimes \Gamma_p + \frac{1}{n} C_S^{(\text{vec})} + o(1/n),$$

with the explicit block

$$C_S^{(\text{vec})} := \sum_{i,j,k,\ell} \sum_{s,t} \left(c_{ij,kl;st}^{(S,\text{bd})} + c_{ij,kl;st}^{(S,0)} + c_{ij,kl;st}^{(S,2)} + c_{ij,kl;st}^{(S,4)} + c_{ij,kl;st}^{(S,6)} \right) \left((e_j \otimes e_i \otimes e_s) (e_\ell \otimes e_k \otimes e_t)^\top \right).$$

Finally, since $\tilde{S}_n = (L_{p+1} \otimes I_p) S_n (L_{p+1} \otimes I_p)^\top$, we obtain $\tilde{S}_n = S_\infty + \frac{1}{n} C_S + o(1/n)$, where $S_\infty = (uu^\top) \otimes \Gamma_p$ and $C_S = (L_{p+1} \otimes I_p) C_S^{(\text{vec})} (L_{p+1} \otimes I_p)^\top$. Absolute summability of $\{\gamma_h\}$ and $\{\psi_k\}$, and finiteness of κ_4, κ_6 , ensure that all series above converge absolutely and justify the $o(1/n)$ remainder. \square

Theorem J.5 (Order of the non-Gaussian gap). *Under Lemma J.4, let $Q = [u/\|u\|, Q_\perp]$ and $P := Q \otimes I_p$. Then the block-inverse expansion of Lemma H.13 applies verbatim, and*

$$\Delta_n = \Gamma_p - \tilde{r}_n^\top \tilde{S}_n^{-1} \tilde{r}_n = \frac{1}{n} B_p + o(1/n),$$

with $B_p \succeq 0$ given by the same closed form as in (9) after replacing the Gaussian C_S, C_r by those from Lemma J.4. Generically $B_p \succ 0$.

Remarks. (i) No Gaussianity is needed for strict PD and the positive Schur-complement gap: independence of innovations with finite fourth moment (and $\text{Var}(\varepsilon^2) > 0$) suffices. (ii) If in addition $\sum_h |\gamma_h| < \infty$ and $\mathbb{E}|\varepsilon|^6 < \infty$, the exact $1/n$ order persists for general linear stationary processes; Gaussianity only simplifies the constants via Wick pairings.

Discussion on AR/MA/ARMA models. Stable AR, MA, and ARMA processes satisfy the assumptions above, so Theorems J.3 and J.5 apply directly. Nevertheless, caution is warranted in interpreting the result. For MA or ARMA models, the one-step prediction error e_{n+1} still carries dependence on portions of the past beyond the last p lags. This prevents a direct characterization of the mean-squared error gap between LSA and linear regression with respect to the true target x_{n+1} . Hence the finite-lag linear regression predictor $\hat{x}_{n+1}^{\text{LR}}$ does not coincide with the globally optimal (infinite-order) linear predictor. In particular, for MA models there may exist richer linear predictors that exploit the entire past more effectively. Our analysis should therefore be understood not as a claim of global optimality across all linear predictors, but rather as an insight into the structural gap that persists even when comparing LSA against the natural p -lag linear regression benchmark.

Auxiliary lemmas used in Appendix J

Lemma J.6 (Moment-cumulant formula). *For random variables X_1, \dots, X_r with finite moments up to order r , the joint moment can be expressed in terms of cumulants as*

$$\mathbb{E} \left[\prod_{i=1}^r X_i \right] = \sum_{\pi \in \mathcal{P}_r} \prod_{B \in \pi} \text{cum}(X_j : j \in B),$$

where \mathcal{P}_r denotes the set of all partitions of $\{1, \dots, r\}$, and $\text{cum}(\cdot)$ denotes the joint cumulant.